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WIMSTAR-4: A COMPUTER PROGRAM FOR GENERATING WIMS LIBRARY DATA FROM ENDF/B

WIMSTAR-4: UN PROGRAMME D'ORDINATEUR DESTINE A PRODUIRE DES DONNEES DE BIBLIOTHEQUE WIMS A PARTIR DE ENDF/B

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RESUME

WIMSTAR (Version 4) est un programme d'ordinateur FORTRAN-IV établi pour produire des fichiers de données pour la bibliothèque de codes de réseaux WIMS à partir de la base de données ENDF/B. On doit utiliser le programme concurrement avec le système AMPX-II. Il a été conçu pour être mis en application comme module de ce système.

Ce rapport décrit la structure, la mise en application et l'emploi du système AMPX/WIMSTAR.

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ABSTRACT

WIMSTAR (Version 4) is a FORTRAN-IV computer program developed to generate data files for the WIMS lattice code library from the ENDF/B data base. The program must be used in conjunction with the AMPX-II system and has been designed for implementation as a module of that system.

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CONTENTS

		<u>Page</u>		
1.	INTRODUCTION	1		
2.	PROGRAM DESCRIPTIONS			
	2.1 GENERAL REMARKS 2.2 AMPX MODULES 2.3 PROGRAM WIMSTAR	3 4 7		
3.	INSTRUCTIONS FOR USING THE PROGRAMS	12		
	3.1 INPUT DECK SETUP 3.2 AMPX MODULE INPUT 3.3 WIMSTAR INPUT 3.4 JOB CONTROL CONSIDERATIONS 3.5 DYNAMIC CORE ALLOCATION 3.6 ERROR PROCESSING	13 14 31 49 50		
4.	PROGRAM MAINTENANCE INFORMATION	52		
	4.1 OVERLAY STRUCTURE 4.2 PROGRAMMING DETAILS 4.3 DATA FILE FORMATS	52 53 55		
5.	SUMMARY			
6.	ACKNOWLEDGEMENTS	67		
	REFERENCES			
	TABLES	70		
	FIGURES	73		

CONTENTS, concluded

		<u>Page</u>
APPENDIX A	WIMSTAR ERROR MESSAGES	75
APPENDIX B	FIDO INPUT SYSTEM	80
APPENDIX C	SAMPLE CASE	88
APPENDIX D	INPUT SUMMARIES	91

1. INTRODUCTION

WIMSTAR* (Version 4) is a FORTRAN-IV computer program developed to generate data files for the WIMS lattice code $^{(1)}$ library tape from the ENDF/B $^{(2)}$ nuclear data system.

Historically, WIMS users have been obliged to accept the library tapes provided by Winfrith (3) with little real control over the contents. The task of checking the data or preparing new data was arduous, time consuming and error prone. WIMSTAR-4, combined with the ENDF processing system AMPX-II (4), now provides a much simplified method of producing the WIMS data files and updating the WIMS library tape.

WIMSTAR-4 is designed to be incorporated as a module of the AMPX-II system, employing the same input conventions, scratch tapes, and dynamic core utilization techniques. Thus in a single computer run it is possible to read the ENDF/B tape, generate the required WIMS data for any nuclide, and place this data into the WIMS library. Inspection and editing facilities are provided for (1) the AMPX-generated point and multigroup cross sections, (2) the WIMSTAR-generated multigroup cross sections and resonance tables, and (3) all data files contained on an existing WIMS tape. In keeping with the design of the AMPX system, each step in the process reads data from one or several input tapes and writes the results to another tape, thus allowing the user to proceed one step at a time verifying, and if necessary correcting, the results before continuing.

WIMSTAR-4 incorporates the linear point cross-section techniques of the TCP system⁽⁵⁾. A module from the RSYST system⁽⁶⁾ is used to solve the slowing-down equation.

^{*} WIMSTAR is an acronym for WIMS TApe Revisor.

The program can calculate all the data required by WIMS with the exception of the fission source spectrum, burnup chains, and χ (used in calculating f(p) in WIMSB; χ is not used in WIMSC or later versions and can be set to zero (7). These data can be taken from the old WIMS tape or created elsewhere and added to the new WIMS tape via the update routine. Several built-in weighting spectra for producing the multigroup cross sections from point data are provided. However, if he prefers, the user can substitute his own, or use the spectra provided by Winfrith. Calculation of the transport cross section supports the methods suggested by Winfrith (8,9,10).

The current version of AMPX-II accesses ENDF/B-IV tapes. When ${\tt V}^{(11)}$ becomes more widely used, AMPX-II and WIMSTAR-4 will be modified accordingly.

WIMSTAR-4 and other modules of the AMPX-II system are currently being run at an IBM installation. Use on another system would be difficult due to the complications in implementing the AMPX system.

Section 2 describes the structure of WIMSTAR-4 and the AMPX-II modules required. Section 3 provides instructions for using the current versions of the programs. Section 4 contains information to aid in making modifications to WIMSTAR-4. Section 5 summarizes the current state of the program and discusses future improvements. Appendix A describes the error messages that may be received when something goes wrong, while Appendix B describes the FIDO input system used by all AMPX modules. Appendix C contains the input for a sample case, and Appendix D provides a convenient summary of the input data and the required tape units.

2. PROGRAM DESCRIPTIONS

2.1 GENERAL REMARKS

The generation of WIMS library data is a multi-step process requiring the execution of three AMPX-II modules: NPTXS, XLACS2, and WIMSTAR-4. Two utility modules, AJAX and RADE, provide useful support and have been included in this discussion. The procedure is illustrated in Figure 1 and briefly explained here. Detailed discussions of each module follow.

Each nuclide on the WIMS data tape has three sets of information. The first is a record describing all the nuclides produced by burnup of this nuclide. This data must be provided to WIMSTAR by the user. The second set contains the basic cross sections at one temperature for the fast and resonance regions, and at one or several temperatures for the thermal region. A resonance nuclide requires a third set of data containing absorption and fission yield (if fissile) cross sections for the resonance region. These cross sections are temperature and concentration dependent, (T, σ_n) , and replace the resonance region cross section of the second set in the WIMS calculations following evaluation of the case data. The creation of the resonance tables requires a point cross-section curve in the resolved resonance region and a curve for each $\sigma_{\mathbf{p}}$ in the unresolved resonance region. These point cross sections are generated by module NPTXS. Module XLACS2 then calculates multigroup cross sections for use in creating the second set above, while module WIMSTAR generates the third set.

Intermediate results are stored in data files external to each module. Through the organization of the AMPX-II system, any number of modules (or segments of WIMSTAR-4) can be executed in one job step.

The steps in generating WIMS data are summarized below.

- Module NPTXS evaluates the ENDF/B resonance parameters to produce point cross sections. File PXS-ID contains resolved resonance region cross sections and infinitely dilute unresolved resonance region cross sections, while file PXS-FD contains unresolved cross sections at several user-selected finite dilutions.
- Module XLACS2 calculates weighted multigroup cross sections in the WIMS energy group structure and writes these to a standard AMPX master library tape.
- Module RADE can be used to check and partially list the data, and module AJAX can be used to edit the data on these master tapes.

Module WIMSTAR-4 performs the remaining steps:

- 4. Segment GXWIMS collects the required data from the ENDF/B tape, the AMPX master library, and the two point cross-section tapes and generates the WIMS library data which are placed on a WIMSTAR data tape.
- 5. Segment WIMLIB then uses the WIMSTAR data tape to update the WIMS library by creating a new WIMS tape.
- 6. Segments TRANS, TAPMAN and SCAN provide listing and editing services for WIMS and WIMSTAR tapes. Segment CONVRT converts WIMS tapes between binary and BCD formats to allow their transfer to other computer centres.

2.2 AMPX MODULES

A brief description of the AMPX modules required is given here. For a detailed discussion please refer to the AMPX-II user's manual (4).

2.2.1 NPTXS

Module NPTXS preprocesses resonance or nonresonance ENDF nuclides to make point files for total, fission, elastic scattering, and (n,γ) cross sections. Several modifications have been made to NPTXS for use with WIMSTAR; thus the user should refer to Section 3.2 of this report and not the AMPX-II user's manual when preparing input for the modified version of NPTXS. These changes involve writing the unresolved cross sections for the σ_p 's* to tape 41 instead of punching them on cards. Also the maximum number of σ_p 's has been increased from 7 to 11.

The resolved resonance region and infinitely dilute unresolved resonance region point cross sections, written to tape 31 (PXS-ID), are used by both XLACS2 (the resonance processing of XLACS2 should be skipped completely), and segment GXWIMS of module WIMSTAR-4. If the nuclide contains unresolved resonance parameters, the data written to tape 41 (PXS-FD, containing unresolved cross sections at several finite dilutions) are used only by GXWIMS.

NPTXS can process both single- and multi-level Breit-Wigner resolved resonance parameters. The resonance data can be Doppler broadened using either the numerical integration techniques of Cullen (SIGMA1 method (12,13)), or the conventional PSI-CHI method. Note that the background ENDF File 3 data will be broadened only by the SIGMA1 method, making it the preferred method. The unresolved processing uses the same techniques as XLACS2, originally developed for the MC-2 code (14). The identification number for the output point cross sections (ID19), input by the user, must be different for each temperature of each nuclide to allow GXWIMS to differentiate between different temperature sets of the same nuclide. NPTXS must be run once for each temperature desired for a given nuclide.

^{*} The σ_p in this report and σ_o in the NPTXS description in the AMPX-II user's manual refer to the same quantity.

2.2.2 XLACS2

XLACS2 is the AMPX module which calculates weighted multigroup neutron cross sections from ENDF/B data. Its calculational routines were originally taken from the SUPERTOG⁽¹⁵⁾ and FLANGE-II⁽¹⁶⁾ codes, and produce full-energy-range neutron cross-section libraries. Provisions are included for treating fast, resonance, and thermal ENDF/B data in a single calculation. Energy group structure and expansion orders used to represent differential cross sections can be averaged over an arbitrary user-supplied weighting function (for example the wet and dry spectra used by Winfrith, Section 3.2) or over any of several built-in weighting functions. The multigroup data produced are written to an AMPX master library tape.

XLACS2 should be directed (through input items MATPT and MATEL of the 71* array, see Section 3.2) to skip all resonance processing and to generate multigroup total, fission, elastic scattering, and (n,γ) cross sections from data on the point cross-section library (PXS-ID) produced by NPTXS.

XLACS2 contains the facility of substituting ENDF/B thermal scattering law $S(\alpha,\beta)$ data in place of normal ENDF/B processing in the thermal energy region (see item MATID of the 70\$ array, Section 3.2). This facility should be used for very light moderators.

XLACS2 should be run once for each temperature desired with the same nuclide identification numbers (item ID19 of the 70\$ array) as were used for the NPTXS data.

2.2.3 AJAX

Module AJAX is used to combine data from AMPX master libraries. Options are provided to allow merging, adding, deleting, or reordering

for any number of input files. AJAX can be used to change the nuclide identification numbers to match the NPTXS data sets if this was not done at the time of generation.

2.2.4 RADE

Module RADE is provided to check the multigroup libraries for consistent and reasonable data. On option, the user can request a display of differential cross sections.

2.3 PROGRAM WIMSTAR

WIMSTAR is organized into six separately executable segments: GXWIMS, WIMLIB, TRANS, TAPMAN, SCAN and CONVRT. Each module is now described.

2.3.1 GXWIMS

There are two phases in the execution of GXWIMS: calculation of resonance tables including Goldstein-Cohen λ values, and calculation of multigroup cross sections.

The resonance integral tables in the WIMS library result from calculations performed with the resonance nuclide under consideration in a homogeneous mixture with hydrogen as the moderator. The table values are a function of both temperature and dilution $(\sigma_p)^{(1)}$. Module RESPU of the RSYST Code System $^{(17)}$ is used to solve numerically the slowing-down equation for the situation of a resonance nuclide mixed homogeneously with hydrogen, using the total and scattering point cross sections provided by NPTXS, and yielding the relative flux, $\phi(u)$. This flux is used to collapse the absorption (and fission yield if the nuclide is fissile) point cross sections

$$\sigma_{RI} = \frac{\int_{u_1}^{u_2} \sigma(u)\phi(u)du}{\int_{u_1}^{u_2} \phi(u)du}$$

into the WIMS multigroup structure. This process is repeated for each σ_p (using the appropriate unresolved resonance region values) and each temperature (using appropriately broadened values).

The Intermediate Resonance (IR) theory of Goldstein and Cohen (18) shows that the resonance integral can be approximated as

$$\sigma_{RI} \sim \frac{1}{\Delta u} \int_{u_1}^{u_2} \frac{\sigma_p}{\sigma_p + \sigma_a(u) + \lambda \sigma_{rs}(u)} \sigma(u) du$$

where σ_{rs} is the resonance scattering cross section and λ is the Goldstein-Cohen parameter taking a value between 0 and 1. A value of 1 produces the Narrow Resonance (NR) approximation, and a value of 0 yields the Infinite Mass (IM) approximation. Using the point cross sections for infinite dilution, GXWIMS attempts to find a value of λ that yields the same resonance integral for absorption as that obtained by solving the slowing down equation. In some cases the IR approximation is not sufficiently accurate to yield a value of λ between 0 and 1 and the user must supply a value manually.

The second phase of GXWIMS obtains the weighted multigroup cross sections from XLACS2 and calculates the following quantities:

$$\sigma_{\mathbf{i}}^{T} = \text{total} = \sigma_{\mathbf{i}}^{a} + \sum_{j} \sigma_{\mathbf{i}j}^{o} - \sigma_{\mathbf{i}}^{n},^{2n}$$

$$\sigma_{\mathbf{i}}^{a} = \text{absorption} = \sigma_{\mathbf{i}}^{T} - \sum_{j} \sigma_{\mathbf{i}j}^{o}$$

$$\sigma_{\mathbf{i}}^{y} = \text{fission yield} = v \sigma_{\mathbf{i}}^{f}$$

$$\sigma_{\mathbf{i}}^{p} = \text{potential scattering}$$

$$\sigma_{\mathbf{i}}^{sd} = \text{slowing down power} = \xi \sum_{j} \sigma_{\mathbf{i}j}^{o} / (u_{\mathbf{i}+1} - u_{\mathbf{i}}).$$

There are several options for calculating the transport cross section $^{(7-10)}$. The recommended procedure is the following:

below 4 eV a row sum correction is applied

$$\sigma_{\mathbf{i}}^{\mathsf{tr}} = \sigma_{\mathbf{i}}^{\mathsf{a}} + \sum_{\mathbf{j}} \sigma_{\mathbf{i}\mathbf{j}}^{\mathsf{o}} - \frac{1}{3} \sum_{\mathbf{j}} \sigma_{\mathbf{i}\mathbf{j}}^{\mathsf{1}}$$

- above 4 eV a weighted column sum correction is applied

$$\sigma_{\mathbf{i}}^{\mathbf{tr}} = \sigma_{\mathbf{i}}^{\mathbf{a}} + \sum_{\mathbf{j}} \sigma_{\mathbf{ij}}^{\mathbf{o}} - \frac{1}{3} \sum_{\mathbf{j}} W_{\mathbf{ji}} \sigma_{\mathbf{ji}}^{\mathbf{1}}$$

where between 4 eV and 9.2 KeV a 1/E current is assumed (i.e. $W_{ij} = \Delta u_i/\Delta u_j$, $\Delta u_i = 1$ ethargy width of group i), and above 9.2 KeV the weights are obtained as $W_{ij} = J_i/J_j$, where $J_i = 1$ neutron current in group i). GXWIMS has no facility to perform these current calculations, thus they must be done elsewhere and the W_{ij} 's input via cards. An alternative option is to assume a 1/E current for all energies above 4 eV. Other options include using the row sum correction for all energies, or simply setting $\sigma^{tr} = \sigma^T$. See Reference 9 for a discussion of the merits of these various transport cross-section options. Finally, for all nuclides on the WIMS tape (except those for which a P_1 scattering matrix is supplied, i.e. hydrogen, deuterium, oxygen and carbon), the self-scattering term of the P_0 matrix is adjusted as

$$\sigma_{ii}^{o} \leftarrow \sigma_{ii}^{o} - \frac{1}{3} \sum_{i} \sigma_{ij}^{1}$$
.

The user must direct GXWIMS as to whether or not this adjustment is required.

GXWIMS then prints and plots the one-dimensional multigroup data for inspection and writes all results to a WIMSTAR data tape.

2.3.2 WIMLIB

Segment WIMLIB reads an old WIMS library tape and, under the direction of user-supplied update and edit commands, uses the results on a WIMSTAR tape to write a new WIMS library tape. New data can be input entirely from the WIMSTAR tape, or entirely from cards, or from a combination of both. A new WIMS tape can be built entirely from scratch if desired. Any entry on the input WIMS tape can be edited, although changing the energy group structure (currently 69 groups) is not permitted. Energy group condensation is a facility that may be added in the future.

2.3.3 SCAN

Segment SCAN reads a WIMS tape, checks for inconsistencies in the structure and "unreasonable" data values, and prints user-selected files. SCAN should be used after every update operation to look for errors and to ensure that the new tape is readable. Only the newly added data need be printed, although the entire tape is checked internally.

SCAN performs the following checks:

- duplicate NIN's (nuclide identification numbers)
- energy boundaries decrease and all unique

- fission spectrum sums to 1.0
- burnup chains in correct order and all NIN's referenced are present
- order of nuclide data files
- check NF, NFA and NZZ for consistency
- count fissiles and fission products and check NNF and NNFP
- thermal data temperatures increase
- erder of RIN's (resonance identification numbers)
- number of tables for each nuclide, NZZ
- NF correct
- T and $\boldsymbol{\sigma}_p$ should increase and all tables same size for each nuclide
- structure of condensed scattering matrices.

SCAN attempts to read the entire tape despite errors encountered. See Section 4.3.1 to interpret the printed data and for a description of the WIMS tape format and meaning of the above variables.

2.3.4 TRANS

Segment TRANS provides a mechanism for transferring data from a WIMS library tape to a WIMSTAR data tape. This operation is useful if it is desired to add another set of data for a nuclide already contained on the WIMS tape, and the user wishes to use the same burnup chain for both entries. An example of this technique is shown in the sample case (Appendix C) for ²³²Th. The alternative is simply to input the burnup chain via cards when running WIMLIB.

2.3.5 TAPMAN

Segment TAPMAN provides editing and listing facilities for WIMSTAR data tapes. Records on a WIMSTAR tape contain values for a specific data type (burnup chain, thermal-smooth, Pl, etc.) for a given nuclide. These records are individually manipulated with TAPMAN allowing the user increased flexibility in handling the data. If segment GXWIMS terminates abnormally and is rerun, some records on the WIMSTAR tape may be repeated. TAPMAN can be used to remove the duplicate copies. Full listings or simply control record summaries can be printed. See Section 4.3.1 to interpret the output.

2.3.6 CONVRT

Segments WIMLIB, TRANS and SCAN handle WIMS tapes in binary format only. If the new WIMS tape is to be sent to another installation, CONVRT is used to convert it to BCD (i.e., card image) format. When receiving a tape from elsewhere, CONVRT converts it back to binary. Two small FORTRAN programs are maintained on cards to perform similar operations at the other computer site. The attributes of the card image tape should be specified as unlabelled, blocked, with fixed-length 80-character records. Seven digits of accuracy are maintained for floating point data.

3. INSTRUCTIONS FOR USING THE PROGRAMS

AMPX-II and WIMSTAR-4 have been implemented on an IBM system. Thus all of the instructions that follow reflect this environment.

3.1 INPUT DECK SETUP

The input data cards required to run each module are grouped in the SYSIN data file as

//GO.SYSIN DD *

module data cards

/*

Each module is initiated by a module request card with an = sign punched in column 1 and the module name following starting in column 2. For example, to initiate XLACS2 use

=XLACS2

Data cards specific to the module follow the module request card. Any number of sets of request card and data cards can be placed in the SYSIN file to execute a series of modules.

All AMPX modules, including WIMSTAR-4, employ the FIDO input system (4). Appendix B contains a user's guide to this system. The input instructions use the following conventions:

- [] indicates the number of input items expected for an array.
- { } indicates conditions under which a block or array is expected to be input.
- () indicates the default value for an item supplied by the program if the item is not input. (The default value is zero if not explicitly indicated.)

If a block is <u>not</u> expected by the program, omit the terminating T as well. If the block <u>is</u> expected but no data arrays are input, the terminating T must still be input. If the { } do not appear for a block or array, that block or array must be input under all conditions, unless explicitly indicated otherwise. See the sample case in Appendix C.

3.2 AMPX MODULE INPUT

3.2.1 NPTXS

Block 1

- 0\$ Broadening Method [1]
 - ID 0 = SIGMA1 method (default).
 1 = PSI-CHI method.
- 1\$ Case Description [1]
 - 1. NNUC number of ENDF nuclides to be processed.
- T Terminate Block 1

Repeat Blocks 2 and 3 for NNUC nuclides.

Block 2

- 2\$ Nuclide Selection Array [6]
 - 1. MATNO ENDF MAT number for nuclide.
 - 2. NDFB unit number for ENDF tape (11).
 - 3. IDTAP 0/1 = no-check/check ENDF library label (1).
 - 4. MODE ENDF library mode, 0/2 = binary/BCD (0).
 - 5. NSIGP number of σ_{D} values (1).
 - 6. ID19 nuclide identification number on point cross-section tapes.

3* Nuclide Options [4]

- RFACT the resolved resonance region energy mesh is based directly on this parameter. Points are chosen such that the ratio of total cross section from point to point is roughly RFACT (0.9).
- SFACT number of practical widths over which the RFACT scheme is used for a particular resonance (10).
- 3. SIGP σ for unresolved calculation. Enter 0 if NSIGP > 1 and use 4* instead (10⁸).
- TDEGIC temperature in Kelvin for Doppler broadening (0).

T Terminate Block 2

Block 3

 ${NSIGP > 1}$

- 4* σ_p array for the unresolved calculation if the number of σ_p 's is greater than 1. Enter σ_p values high to low, maximum number is 11. [NSIGP]
- T Terminate Block 3

End of Data

Notes:

- 1. The σ_p in this report and σ_o in the AMPX-II user's manual both refer to the potential scattering cross section. See the definition for SIG in XLACS2 array 71*, and the definitions of SIGPA and σ_p in GXWIMS arrays 3* and 5* respectively.
- A reasonable range for RFACT is 0.7 to 1.0. If the input value is outside this range, NPTXS resets it to the default value.

- 3. If NSIGP = 1, the desired σ_p is input in the 3* array, and Block 3 array 4* is not required.
- NPTXS is run once for each temperature, changing the value of ID19,
 2\$ array, each time.
- 5. File requirements:

ENDF library type (input)
PXS-ID tape, unit 31 (output)
PXS-FD tape, unit 41 (output)
scratch units 14, 15, 16, 17, 18, 19.

Input instructions for the remaining AMPX modules, XLACS2, AJAX and RADE, are taken directly from the AMPX-II user's manual (4).

3.2.2 <u>XLACS2</u>

Block 1

Five title cards, each in (20A4) format. The five cards of Hollerith information can be used to describe the neutron library being produced. The block terminator is <u>not</u> input.

Block 2

- 1\$ General Problem Information [5]
 - ID Identification number for the neutron library. Any number will suffice. This number is carried as a user identifier on the library, but is not actually used by any module in AMPX.
 - 2. NNUC Number of ENDF materials to be processed.
 - 3. MAXG Total number of neutron energy groups.
 - 4. NEG Number of thermal neutron energy groups.

- 5. IW Weighting option trigger.
 - 1 Fission-constant-Maxwellian⁺
 - 2 Fission-1/E-Maxwellian+
 - 3 1/(σ_TE); each material has a unique weighting function determined from the point values of the total cross section of the material. (This option should not be used for resonance nuclides. Instead, the IW=5 option is provided for 1/(σ_TE) weighting of resonance nuclides.)
 - 4 Fission-arbitrary-Maxwellian⁺. The arbitrary weighting function is input in the 5% and 6* arrays.
 - 5 $1/(\sigma_T^E)$ where $\sigma_T^{}$ is read from a point cross-section library which was produced by the AMPX module NPTXS. The logical unit for the point cross-section library and the identification number for the point data set to be used are specified in the 71* array.
 - 6 Fission-arbitrary-Maxwellian⁺. The arbitrary function is read from an existing library of weighting functions residing on logical unit 46. The arbitrary function is selected with the NPE parameter in the 2\$ array.
 - 7 $1/[E(\sigma_T + \sigma_p)]$ where σ_p is the SIGP parameter of the 71* array and σ_T is read from a point cross-section library produced by NPTXS. The logical unit for the point cross-

⁺ The weighting spectrum is a composite spectrum composed of a fission spectrum in the high energy range, a constant, 1/E, or arbitrary spectrum (IW=1, 2, 4 or 6) in the intermediate energy range, and a Maxwellian spectrum in the low energy range. The energies at which the three spectra are joined, the temperature of the Maxwellian spectrum, and the fission spectrum temperature are specified in the 8* array. Note that a constant, 1/E, or arbitrary spectrum can be specified for the entire problem energy range by using the appropriate entries in the 8* array to place the Maxwellian spectrum below the problem energy range, and/or to place the fission spectrum above the problem energy range.

section library and the identification number for the point data set to be used are specified in the 71* array.

2\$ Secondary Problem Information [12]

{This array is required only if one or more of its elements is different from the default value shown in parentheses.}

- 1. LSLAB Not used (0)
- 2. LCYL The maximum number of points contained in any of the ENDF/B File 3 arrays. (5 250) If the MATPT or MATEL entries in the 71* array specify that NPTXS-produced point cross-section data are to be used, arrays dimensioned by LCYL may need to be increased to accommodate the point data. Consequently, LCYL must be the maximum of the following: (1) 5 250, (2) number of points in the weighting function specified by IW+250, (3) maximum (number of points from MATPT or MATEL data set for MT=1, 2, 18, or 102 data) + 250. The number of points in the weighting function specified by IW is as follows:

IW	Number of Points		
0, 1, 2, or 3	Assume 2 000		
4	MCSM (2\$ array)		
5 or 7	Number of points in MATPT data set for MT=1		
6	Maximum number of points in any of the arbitrary weighting functions on logical unit 46.		

3. LUNR - The dimension of an array used in conjunction
with cross-section weighting. (10 000) If
NPTXS-produced point cross-section data are to
be used, arrays dimensioned by LUNR are also
used to accommodate the point area. Consequently,

LUNR must be the maximum of 10 000 or the following:

{(2 x number of points in weighting function) + [2 x maximum (number of points from point library for MT = 1, 2, 18, or 102 data)] + 700}

The number of points in the weighting function is described above.

- 4. MSN The maximum number of interpolation regions needed to describe any ENDF/B File 3 array or to describe any TAB1 record produced in XLACS2. (250). (To date, the default value has been adequate for all XLACS2 problems run.)
- 5. NPE Identification number of arbitrary function.
 This entry required only if IW = 6. (0)
- NPEP Logical unit for XLACS2-produced master crosssection library. (23)
- 7. IDTAP Number of reactions for which cross sections are to be punched. ENDF/B File 3 cross sections averaged by XLACS2, multigroup representation of the weighting function, χ, etc., can be punched in free-form FIDO format. Data to be punched are identified in the 4\$ array. (0)
- MODE Format of the ENDF library on logical unit NGMA. (0)
 - 0 Binary-formatted library
 - 1 BCD-formatted library
- 9. NGMA Logical unit number of the device which contains ENDF/B neutron cross-section data, i.e., the ENDF library. (11) Data for the thermal energy range may or may not be on this device.

(The 6th, 7th, and 9th entries of the 70\$ array are used to identify the thermal data when the fast and thermal data reside on separate devices.)

- 10. LCSM If IW ≠ 4, enter 0. If IW = 4, enter the number of regions used to specify the arbitrary weighting function in the 5\$ array. (0)
- 12. NDNP Not used. Enter 0. (0)
- 3\$ Six triggers, IØPT(i), to specify amount of printed output desired.
 [6]

i	IØPT(i) Correspondence	Value***			
		0	1_	2	3
1	Resolved and unresolved resonance processing			formats le)	*
2	Averaged cross sections by energy group and process	formats	formats	PMX icab for	l o
3	Elastic scattering matrices	effect	AMPX	in A appl	ient
4	Thermal scattering matrices	Ν̈́	in A	data* 0 (if	convenient as process
5	Inelastic scattering matrices		Edit	Pg dε	in co
6	(n,2n) scattering matrices		, ,	Edit I l	Edit j

^{*} The P_0 data, if applicable, are edited with an IØPT (i=1); a value of 2 includes the P_0 data.

Т

^{**} The terminology "convenient" is used to imply a convenient form from a programming viewpoint.

^{***} The default value for IOPT(i) is zero.

Terminate Block 2

Block 3

- 4\$ ENDF MT identifiers of the reactions for which cross sections are to be punched. [IDTAP]
- 5\$ If IW = 4, enter the interpolation schemes for the arbitrary weighting spectrum, i.e., (NBT(i), INT(i), i=1,LCSM). [2LCSM]. Standard ENDF/B conventions for the meaning of NBT and INT must be followed—see Reference (2).
- 6* If IW = 4, enter the arbitrary weighting spectrum, i.e., (E(i),W(i), i=1,MCSM) [2*MCSM] E(i) units are eV's. W(i) units are per unit energy. Entries should be low-to-high in energy. The relation between 5\$ and 6* arrays is described in Reference (2). The spectrum used by Winfrith is shown in Table 1.
- 7* Energy Group Boundaries. [MAXG+1] The group boundaries are input (high-to-low) in eV. Many "standard" group boundaries are available in a library that is available with the AMPX package--the "built-in" group structure library. When a "standard" group structure is desired, the 7* array can be omitted. The group structure library received with the AMPX-II package has been modified for the present implementation to include the WIMS 69-group structure illustrated in Table 2.
- 8* Weighting Option Specifications. [10] The 8* array is obtained by default only if IW = 1, 2, 4, or 6. The array is used to specify the energies where the Maxwellian and/or fission spectra are joined to the intermediate-energy-range weighting spectrum and to specify the temperatures of the Maxwellian and fission spectra.
 - 1. T temperature in K for Maxwellian spectrum. (300)
 - 2. χ a multiplier on kT where a join to next portion of weighting spectrum and the Maxwellian is made. (5) Note

that k is Boltzmann's constant ($k = 8.6275 \times 10^{-5}$ eV/K); therefore, 5kT = 0.1264 eV. The Maxwellian spectrum is placed in the region below χkT .

- 3. THETA- fission spectrum temperature. $(1.27 \times 10^6 \text{ eV})$
- 4. FCUT point at which a fission spectrum is joined to spectrum selected by IW. $(67.4 \times 10^4 \text{ eV})$ The fission spectrum is placed in the region above FCUT.
- Not used enter zero. (0)
- 6. Not used enter zero. (0)
- 7. Not used enter zero. (0)
- 8. Not used enter zero. (0)
- 9. Not used enter zero. (0)
- 10. Not used enter zero. (0)
- T Terminate Block 3. (Note that if none of the arrays in Block 3 is entered, a T must still be entered.)

The data for the NNUC ENDF materials to be processed are stacked one set after the other. A "set" of data for a nuclide consists of a title card and Blocks 4 and 5 as follows:

Title Card-(20A4) format.

This card is a title card for the nuclide. The title will be carried throughout AMPX with the neutron cross sections. The first 48 characters will be used as a title for ANISN cross-section sets subsequently produced by the NITAWL module.

Block 4

70\$ Nuclide General Information [9]

- ID19 The identification number for this nuclide. This
 number is carried as the identifier of the data on
 the master neutron cross-section library produced by
 XLACS2.
- MATNO The ENDF/B material number (MAT number) of the set of data to be processed (fast data).
- 3. NTEMP For multithermal groups, NEG > 1, NTEMP is the number of temperatures at which a thermal scattering kernel will be calculated. Doppler broadening is included in the resonance treatments, but only at the first temperature specified in the 73* array. To Doppler broaden a resonance material in a one-thermal-group calculation at a temperature other than the default value of 300K, set NTEMP = 1 and input the temperature in the 73* array. Caution: setting NTEMP = 0 in a multithermal group calculation results in a temperature of 0 K being used and provides no downscatter data in the thermal range. (0)
- 4. LORDER Order of expansion for the scattering matrices above thermal. Elastic scattering and all inelastic levels (MT=51-90) will have matrices of this order.

 (0)
- 5. NL If NEG > 1, enter the order of expansion for the thermal scattering matrices. (0)
- NFY If NEG > 1 and if thermal ENDF data are to be mounted on KMXA, identify the format of the data as follows:
 0 Binary formatted data
 2 BCD formatted data
 The default value is zero.
- 7. MATID The meaning of this parameter depends on the value of NEG and the presence of thermal data on KMXA as follows:

NEG	Thermal Data on KMXA	MATID	
<u><</u> 1	N/A	Enter zero	
> 1	Yes		ication number (MAT number) ta $S(\alpha,\beta)$ data if
> 1	No	Parameter serves as a trigger for an analytic free gas calculation. The free gas kernel is generated using routines from the THERMOS ⁽¹⁹⁾ code. The value of MATID depends on the atomic weight of the material being processed as follows:	
Atomic Weight		Recommended MATID	Remarks
	<u><</u> 19	0	Causes $S(\alpha,\beta)$ "free gas" data to be generated from which P_{ℓ} (order NL) matrices are produced
	no resonances nermal range	-1	A P_0 analytic free gas kernel is calculated
	resonances in mal range	-2	A P ₀ analytic free gas kernel is calculated and normalized to the ENDF/B File 3 elastic data

8. .KMXB - If NEG > 1, enter the number of atoms per molecule of principal scatterer for which the $S(\alpha,\beta)$ data in File 7 of the ENDF data set apply. For example, hydrogen is the principal scatterer in water and has two atoms per molecule; therefore, KMXB = 2.

> 19

> 19

⁺ Examples of thermal ENDF data sets are H bound in $\rm H_2O$ (MAT 1002), D in $\rm D_2O$ (1004), C in graphite (1065), C in $\rm CH_2$ (1011), Be (1064), $\rm C_6H_6$ (1095), H in ZrH (1096) and Zr in ZrH (1097).

- 9. KMXA If NEG > 1, enter the logical unit number of the device which contains the thermal data (MATID) -if not the same device as NGMA.
- 71* Resonance Information [9] {Needed for a resonance nuclide only }
 - 1. SIG σ_p, the potential scattering cross section in barns per atom of the resonance nuclide for a nuclide (or mixture of nuclides) which is admixed with the resonance nuclide in a homogeneous system, is defined as follows:

$$\sigma_{p} = \frac{\sum_{j=1}^{M} N_{j} \sigma_{sj}}{N_{D}}$$

- where N_{j} is the number density of the jth component of the mixture in atoms/barn-cm.
 - $\mathbf{N}_{\mathbf{D}}$ is the number density of the resonance nuclide in the mixture.
 - in the resonance region for the jth component in barns/atom.
- M is the number of components in the mixture. The default value of σ_p is 1.0 x 10^8 , and is the recommended value for the WIMSTAR application.
- 2. AJIN The l = 0 j-state for which unresolved parameters will be passed to NITAWL. The NITAWL unresolved treatment is restricted to one unresolved sequence.

⁺ For the infinite dilution case, $\sigma_p = \infty$. This can be approximated by $\sigma_p = 1.0 \times 10^8$.

A table of scattering cross sections is given in Table IV-1 of Reference (20).

The "most important" sequence should be identified and passed via this input parameter. The resonance with the smallest mean level spacing is usually the "most important".

3. RFACT - The r-factor in the Nordheim (21) resolved resonance treatment. This factor is used to determine the integration mesh spacing (lethargy) through

$$\epsilon_1 = (\Gamma_{D_0}/rE_0),$$

where ϵ_1 is the mesh size, Γ_{D_0} is the Doppler width at 273 K, and E_0 is the resonance peak energy. A value of 5.0 has been found adequate for most cases. (5.0)

- 4. SFACT The s-factor in the Nordheim resolved resonance treatment. This is the number of practical widths on either side of a resonance peak to which the Nordheim treatment is applied. A value of 5.0 has proven sufficient. (5.0)
- 5. MATPT The meaning of this parameter depends on the value of IW as follows:

IW Meaning of MATPT

- 5 or 7 Enter the identification number (usually the ENDF MAT number) of the point data set on logical unit NUNIT used for the $\sigma_{\rm T}$ in the weight function. (Point data sets are usually produced by the NPTXS module.)
- \neq 5 or 7 To bypass all resonance processing for a resonance nuclide, enter the identification number of the point data set on logical unit NUNIT. The $\sigma_{\rm el}, \ \sigma_{\rm f},$ and $\sigma_{\rm n,\gamma}$ data are taken from the point data set, and the corresponding ENDF File 2 and File 3 data for

MATNO are ignored. The ID19 master data set will contain no resonance parameters. (Consequently, NITAWL can do no further resonance processing.)

- # 5 or 7 For a resonance nuclide, enter zero to trigger XLACS2 to do the unresolved resonance processing and to place resonance parameters in the master data set for subsequent resolved resonance processing by NITAWI...
- # 5 or 7 For a non-resonance nuclide, set MATPT equal to
 zero.

Default value for MATPT is zero (0).

- 6. NUNIT If MATPT and/or MATEL ≠ 0, enter the logical number of the device which contains the point cross-section library. Otherwise, enter zero. (0)
- 7. MME Number of angles for the Lobatto quadrature used in the calculation of the elastic scattering transfer array. The default value (0), which causes XLACS2 to calculate an MME based on the mass of the nuclide, is generally adequate.
- 8. MMI Number of angles for the Lobatto quadrature used in the calculation of the inelastic scattering transfer array. The default value (0), which causes XLACS2 to calculate an MMI based on the mass of the nuclide, is generally adequate.
- MATEL Elastic scattering processing trigger for resonance nuclides.

- O Prepare elastic scattering data from the ENDF/B data on logical unit NGMA.⁺
- MAT- Use the MT 2 data for data set MAT on the point cross-section library (logical unit 31) to prepare the elastic scattering cross sections.

T Terminate Block 4

Block 5 {Required only if NTEMP > 0}

- 73* Temperature(s) at which to evaluate the thermal scattering kernel.

 [NTEMP] Temperature(s) in K is/are input low-to-high. Only one temperature should be input for the WIMSTAR application.
- T Terminate Block 5

End of Data

Notes:

1. XLACS2 is run once for each temperature desired, changing the value of ID19, 70\$ array, each time. Use the same values of ID19 that were used in NPTXS. NTEMP, 70\$ array, should be set to 1 and the one temperature value entered in the 73* array. XLACS2 can be rerun several times by setting NNUC, 1\$ array, to the number desired and changing the temperature for each rerun.

⁺ For a resonance nuclide, the XLACS2 resolved resonance processing produces average elastic scattering data in 81 equal lethargy panels per energy group. If MATEL = 0, these data are used to prepare the elastic scattering matrices. However, an alternative (more accurate) procedure for calculating elastic scattering transfer matrices is available. The alternative procedure is triggered by setting MATEL equal to the identification number of a data set in an NPTXS-generated point cross-section library on logical unit NUNIT. XLACS2 will bypass the use of internally generated elastic scattering data and will use the MT 2 data from the point cross-section library.

2. File requirements:

ENDF/B fast library, unit 11 (input)
ENDF/B thermal library, unit 12 (input)
AMPX master library, unit 23 (output)
AMPX group structure library, unit 47 (input)

3.2.3 AJAX

Block 1

- 0\$ Logical Assignments [2]
 - 1. MMT Unit no. of new library. (1)

scratch units 14, 15, 16, 17, 18.

- NMAX Unit no. of the input file which has the largest buffer requirements.
- 1\$ Number of Files [1]
 - NFILE No. of file requests to be made. When reordering
 operations are performed which require the same file
 to be accessed several times, each access is counted
 to determine NFILE.
- T Terminate Block 1

Blocks 2 and 3 are repeated NFILE times.

Block 2

- 2\$ File and Option Selection [2]
 - NF Unit no. of input library.
 - 2. IOPT option
 - N = delete N nuclides from NF to create new library on MMT.

- 0 = add all nuclides on library MMT.
- + N = add N nuclides from NF to create new library on MMT.

Note:

Sets with duplicate identifiers will not be entered on MMT. The first occurrence of an identifier selects that set for the new library.

T Terminate Block 2

Block 3 {Enter only if IOPT ≠ 0}

- 3\$ List of nuclide identifiers to be added or deleted from NF. [/IOPT/]
- 4\$ List of new identifiers. This array allows changing of the identifiers given in 3\$ array when selecting nuclides for new library.

 {Enter only if identifiers are to be changed} [/IOPT/]
- T Terminate Block 3

End of Data

Note:

1. File requirements:

AMPX master library tape (output)

AMPX master library tape(s) (input)

scratch units 15, 16, 18, 19.

3.2.4 RADE

Block 1

- 1\$ Checking Commands [4]
 - 1. MMT AMPX master library unit no.
 - MWT
 MAN
 not required for WIMSTAR applications, enter zeroes.
 - 4. IFM

2\$ Options [20]

- 1. IOPT1 no. of angles at which a display of differential cross sections is desired. These angles will be equally spaced in the cosine range -1 to 1.
- 2. IOPT2 the accuracy in 1/1000's of a percent to which checks are made (e.g., 1 = 0.001%). (1)
- 3. IOPT3

 not used, enter zeroes.

 20. IOPT20
- T Terminate Block 1

End of Data

Notes:

- RADE can also check ANISN libraries. Although this option is not required for the WIMSTAR application, the user can refer to the AMPX-II user's manual (4) for details.
- 2. File requirements:

AMPX master library tape (input) scratch units 18, 19.

3.3 WIMSTAR INPUT

Module WIMSTAR is requested via the

=WIMSTAR

module request card. Each segment of WIMSTAR is initiated via a segment request card which has the segment name punched starting in column 1. The rest of the card is read and printed as a title for the segment listing. For example:

GXWIMS- CALCULATE TH-232 WIMS DATA AT 300 K

initiates segment GXWIMS. The FIDO input data cards follow each segment request card. See the sample case in Appendix C.

3.3.1 GXWIMS

Block 1

- 1\$ Run Counter [1]
 - NNUK No. of nuclides to be processed.
- T Terminate Block 1

Sets of Blocks 2 though 6 are repeated NNUK times.

Block 2

- 2\$ Run Parameters [16]
 - NDF ENDF/B tape unit no.
 - NWD WIMSTAR tape unit no.
 - IOUT Output print flag:
 - 0 = partial print (including all WIMS data)
 - 1 = full print (of NAM contents).
 - 4. IDTAPE Identification no. of the new WIMSTAR tape. If IDTAPE = 0, an existing tape is assumed and the data is added to the end.
 - MAT ENDF/B material no.
 - IDN WIMSTAR nuclide identification no.
 - 7. NTE No. of temperatures to be processed, maximum of 10.
 - 8. NSP No. of σ_p values in the resonance calculation, $\label{eq:nsp} \text{NTE} \, + \, \text{NSP must be} \, \leq \, 20 \, .$

- 9. NG No. of groups. (69)
- 10. N1 No. of fast groups. (14)
- 11. N2 No. of resonance groups. (13)
- 12. N3 No. of thermal groups. (42)
- 13. IFL Smooth data calculation flag:
 - 0 = nc
 - 1 = yes, but don't perform the λ calculation
 - 2 = yes, including λ calculation.
- 14. IFR Resonance table calculation flag:
 - 0 = no resonance tables
 - 1 = σ_a tables only, no σ_p tape data
 - 2 = σ_a and $v\sigma_f$ tables only, no σ_p tape data
 - $3 = \sigma_a$ tables, including σ_p tape data
 - 4 = σ_a and $v\sigma_f$, including σ_p tape data.
- 15. IFP Aux. input from Block 5:
 - 0 = no
 - 1 = yes
- 16. NWK Size of the auxiliary work spaces. (500)
- T Terminate Block 2

Block 3

- 3* Calculation Parameters [5]
 - 1. DUMAX Maximum lethargy difference.

$$\Delta u_{\text{max}} = \frac{2}{3} (1-\alpha)$$

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$

A = atomic no. of nuclide

This is calculated internally if DUMAX = 0.0 is entered.

- 2. SIGPA Average potential scattering cross section of absorber. {Required only if IFR > 0.}
- AWA Atomic weight of absorber.
- 4. APA Effective scattering radius in units of 10⁻¹² cm from ENDF/B file 2 data⁽²⁾. If APA is entered as 0.0, the program takes the value from the ENDF/B tape.
- 5. ERR Relative interpolation error used in processing point cross sections. (0.001)
- 4* List of temperatures, increasing order. [NTE]
- 5* List of σ_p values for resonance calculation, increasing order. {Required only if IFR > 0.} [NSP]
- T Terminate Block 3

Block 4 {Repeat NTE times }

- 6\$ Temperature-Dependent Parameters [8]
 - ID19 AMPX nuclide identification no., must be different for each temperature.
 - NAM AMPX master library tape unit no. from XLACS2 module of AMPX.
 - 3. NXS Tape unit no. of point cross-section tape (PXS-ID) created by NPTXS module of AMPX. {Only if IFR > 0.}
 - 4. NSD Tape unit no. of tape created by NPTXS module of AMPX containing unresolved point cross sections for each $\sigma_{\rm D}$ in 5* array (PXS-FD). {Only if IFR > 2.}
 - 5. ITFP Data plot flags: (1)
 - 0 ≈ no plotting
 - 1 = plot WIMS data
 - 2 = plot WIMS data and point curves for $\sigma_{\rm T}(u)$, $\sigma_{\rm q}(u)$ for resonance calculation

```
3 = same as 2 including \phi(u)
```

- 6. ITFT Transport cross section calculation: (2)
 - $0 = use \sigma_m$
 - 1 = use row sum method
 - 2/3/4/5 = use row-column sum method with weight
 factors: lethargy widths/read from 9* array/
 previous weights read/previous weights read
 with changes from 9* array.
- 7. ITFO P self-scattering term adjustment:
 - 0 = yes
 - 1 = no
- 8. ITF1 P, output to NWD:
 - 0 = no
 - 1 = yes
- T Terminate Block 4

Block 5 Aux. Input {Only if IFP = 1 }

- 7* List of λ values to be used if λ -calculation is not performed or fails to generate a usable value. [N2]
- 8* Energy structure (high to low, eV). {Used only if IFL = 0 and no AMPX master libraries are used.} [NG + 1]
- T Terminate Block 5

Block 6 {Repeat for each occurrence of ITFT = 3 or 5 }

- 9* List of weighting factors for calculating σ_{tr} for the fast groups ordered "to" (1 \rightarrow N1) within "from" (1 \rightarrow NG). [NG*N1]
- T Terminate Block 6

End of Data

Notes:

- 1. Sets of Blocks 2 through 6 are repeated NNUK times.
- For each occurrence of Block 4 after the first (for any given nuclide), only the values of the parameters that change must be input. ID19 must change for each temperature.
- 3. IOUT only controls listing the data read from the AMPX master library tape and produces considerable output. It should be set to l only if problems develop or the data is suspected to be inaccurate.
- 4. For ITFT = 4 or 5, only weights read previously for this nuclide can be accessed as the resonance calculation uses the same work tape that the weights are stored on, and are thus overwritten. Weights are input ((W_{ij}, i=1,N1), j=1,NG) where i ranges over the fast "to" groups and j over all "from" groups. See Section 2.3.1 and Reference (9).
- 5. File requirements:

AMPX master library tape(s) (input)

NPTXS point cross section tape(s) (input)

ENDF/B tape (input)

WIMSTAR data tape (output)

scratch units 14, 15, 16

6. If this nuclide is hydrogen, deuterium, oxygen or carbon, both ITFO and ITF1 should be set to 1; set to 0 otherwise.

3.3.2 WIMLIB

Block 1

- 0\$ Output Print Flag [1]
 - TOUT Controls printing of edited WIMS data. 0/1 = No/Yes.
 The 0\$ array may also be entered in Blocks 3, 5, 8, and 11, thus allowing the print to be switched on and off as required.

1\$ Run Parameters [8]

- NWO Old WIMS tape unit no. {Not required if all input from NWD or cards.}
- 2. NWN New WIMS tape unit.
- 3. NWD WIMSTAR Data tape unit. {Not required if all input from NWO or cards.}
- 4. LRIN No. of resonance tables on new WIMS tape.
- 5. NEB No. of burnup chain edits.
- 6. NES No. of nuclide data file edits.
- 7. NER No. of resonance table edits.
- 8. NEP No. of Pl matrix edits. Must be either 0 or 4.

2\$ New WIMS Tape Control Record [8]

- 1. LNIN No. of nuclides.
- 2. NG No. of energy groups, NG=N1+N2+N3. (69)
- 3. NO No. of groups into which there is fission source. (27)
- 4. N1 No. of fast groups. (14)
- 5. N2 No. of resonance groups. (13)
- 6. N3 No. of thermal groups. (42)
- 7. NNF No. of fissile nuclides.
- 8. NNFP No. of fission product nuclides.

Warning: NG, N1, N2, N3 are included only for completeness of edit facilities; the program cannot change the group structure.
These values must be identical to the old WIMS tape values.

T Terminate Block 1

Block 2

- 8\$ List of nuclide identification numbers (NIN's) to be placed on new WIMS tape. [LNIN]
- 9* List of resonance table identification numbers (RIN's) to be placed on new WIMS tape. [LRIN]

Note 1:

Arrays 8\$ and 9* define the data to be placed on the new WIMS tape. Any data on the old tape but not in these lists will be deleted. RIN's must be in same order as NIN's, which must be in the same order as the old tape. New NIN's can be placed in any order on the new tape.

Note 2:

In the following description, arrays marked with an underscore (e.g., 10*) are used for both data input and data edit. If the data is input from an old WIMS tape or a WIMSTAR data tape, these arrays are required only if changes are necessary. Standard FIDO commands are used to access selected values. In some cases the length of these arrays is entered on cards. These values are only used if the complete array is input via cards. If input is via old WIMS tape or WIMSTAR tape, the length cannot be changed via card input.

- 10* Energy group boundaries. [NG+1]
- 11* Fission source spectrum. Sums to 1.0. [NO]
- T Terminate Block 2

$\underline{Block\ 3} \qquad \{NEB > 0\}$

- 3\$ Burnup Chain Edit Control [3]
 - NIN3 NIN of nuclide to be edited. Order must match NIN list of 8\$ array.
 - 2. ID3 Data source:
 - < 0 old WIMS tape

- = 0 card input
- > 0 WIMSTAR tape, ID3 is identification no. of the data.
- 3. LENB Length of burnup chain. {Required only if ID3 = 0.}
 If ID3 ≠ 0, LENB is used to indicate the negative of the no. of chain edits entered in 14*. For example, if ID3 < 0 and 3 edits are required, enter LENB = -3.</p>

T Terminate Block 3

Block 4 {NEB > 0}

- 10* Burnup chain for NIN3. The first two words of the chain are replaced by LENB and NIN3 respectively, and should be entered as zero.
 [LENB]
- 14* Burnup chain edit control. A set of 3 entries is input for each edit operation as follows:
 - 134 1.2-2 2135 NIN2135 is added for the chain after NIN134, with yield 1.2E-2,
 - 134 0.0 0 NIN134 is deleted.

The length of the chain is adjusted internally. The first eight entries in the chain cannot be modified via the 14* array; the 10* array is used for this. Changes via the 10* array are completed before those of the 14* array. {Only if LENB < 0, ID3 \neq 0.} [|LENB|x 3]

T Terminate Block 4

Sets of Blocks 3 and 4 are repeated NEB times.

Block 5 {NES > 0}

- 4* Nuclide Data File Edit Control [9]
 - NIN4 NIN of nuclide to be edited. Order must match NIN list of 8\$ array.

- 2. ID4 Data source:
 - < 0 old WIMS tape
 - = 0 card input
 - > 0 WIMSTAR tape, ID4 is identification no. of data.
- 3. TFR Temperature of fast and resonance data.
- 4. AW Atomic weight.
- 5. IAN Atomic number.
- 6. NF Fissile-resonance table trigger:
 - 0 = non-fissile, no res. tables
 - 1 = non-fissile, res. absorption tables
 - 2 = fissile, res. absorption tables
 - 3 = fissile, res. absorption and fission yield
 tables
 - 4 = fissile, no res. tables
- NT No. of temperatures at which thermal data is tabulated.
- 8. NZZ No. of resonance tabulations.
- 9. NP4 Length of condensed PO scattering matrix. {Required only if ID4 = 0.}

Note:

Items 4 - 8 are required only if $ID4 \ge 0$. If ID4 < 0, they are taken from the old WIMS tape unless overridden via 4* array; e.g., addition of a new resonance table would require increasing NZZ of old tape.

T Terminate Block 5

Block 6 {NES > 0}

- 12* Transport cross section, σ₊₊. [N1+N2]
- 13* Absorption cross section, σ₂. [N1+N2]
- 14* Chi, χ , not used in WIMSC or later versions. GXWIMS places zeros in this array which can be overwritten using cards if desired.
 [N2]
- 15* Goldstein-Cohen parameters, λ . [N2]
- 16* Fission yield cross section, $v\sigma_f$. {Required only if NF \geq 2.} [N1+N2]
- 17* Fission cross section, $\sigma_{\rm f}$. {Required only if NF \geq 2.} [N1+N2]
- 26* PO condensed scattering matrix from fast and resonance groups.
 [NP4]
- 23* Temperatures for thermal data tabulations. The number and values of the temperatures may be different from the old WIMS tape.

 However, if this is the case, all thermal data must be replaced. In other words, if ID4<0, NT must equal NT of old tape and 23* is not required; if ID4>0, 23* is necessary. [NT]
- 24\$ Length of thermal PO scattering matrix for each temperature. {Required only if ID4=0.} [NT]
- 25\$ Thermal edit flags. NT entries corresponding to each thermal temperature, 0 = no edit or input, 1 = edit or input. Block 7 is input for each 1 in 25\$ array. [NT]
- T Terminate Block 6
- Block 7 {Repeat for each 1 in 25\$ array and NES > 0 }
- 18* Transport cross section, σ_{tr} . [N3]
- 19* Absorption cross section, og. [N3]
- 20* Fission yield cross section, $v\sigma_f$. {Required only if NF ≥ 2 .} [N3]
- 21* Fission cross section, σ_f . {Required only if NF \geq 2.} [N3]

- 26* PO condensed scattering matrix from thermal groups. [Entries in 24\$ array.]
- T Terminate Block 7

Sets of Blocks 5, 6 and 7 are repeated NES times.

Block 8 {NER > 0}

- 5* Resonance Table Edit Control [5]
 - RIN5 RIN of nuclide to be edited. Order must match RIN list of 9* array.
 - 2. ID5 Data source:
 - < 0 old WIMS tape
 - = 0 card input
 - > 0 WIMSTAR tape, ID5 is idendification no. of data.
 - 3. ISF Cross section type:
 - 1 = Absorption
 - 2 = Fission yield. (1)
 - 4. NTE No. of temperatures. {Required only if ID5 = 0.}
 - 5. NSP No. of σ_p values. {Required only if ID5 = 0.}
- T Terminate Block 8

Note:

Each resonance file contains one (absorption) or two (absorption and fission yield) records for each resonance tabulation, depending on NF in the nuclide data file of the nuclide to which the tabulation refers. If a nuclide contains a fission yield tabulation and is to be edited, two sets of Blocks 8, 9 and 10 are required; the first edits absorption (ISF=1) and the second edits fission yield (ISF=2), both with the same value of RIN5. Each set counts towards the total NER.

Block 9 {NER > 0}

- 10\$ Group edit flags. N2 entries, 0 = no edit, 1 = edit, corresponding to each of the N2 resonance energy groups. Block 10 is input for each 1 in 10\$ array. [N2]
- 11* List of temperatures, increasing order. {Required only if ID5 = 0.}
 [NTE]
- 12* List of σ_p values, increasing order. {Required only if ID5 = 0.} [NSP]
- T Terminate Block 9
- Block 10 {Repeat for each 1 in 10\$ array and NER > 0 }
- 13* Resonance cross sections (absorption or fission yield depending on whether this is the first or second tabulation). Ordered σ_p within temperature. [NTExNSP]
- T Terminate Block 10

Sets of Blocks 8, 9 and 10 are repeated NER times.

Block 11 {NEP > 0}

- 6\$ P1 Scattering Matrix Edit Control [1]
 - ID6 Data source:
 - < 0 old WIMS tape
 - = 0 card input
 - > 0 WIMSTAR tape, ID6 is identification no. of data
- T Terminate Block 11

Block 12 {NEP > 0}

- 10* Pl scattering matrix, ordered "to" groups within "from" groups.
 [NGxNG]
- T Terminate Block 12

Sets of Blocks 11 and 12 are repeated NEP times.

Note:

There are four P1 matrices on a WIMS tape, one each for hydrogen, deuterium, oxygen and carbon, in that order. If NEP = 0 they are copied from old to new tape directly and Blocks 11 and 12 are not required. If NEP = 4, each is edited in turn.

End of Data

Notes:

1. File requirements:

WIMS tape (input)

WIMS tape (output)

WIMSTAR data tape (input)

scratch units 14, 15

3.3.3 SCAN

Block 1

- 1\$ Run Parameters [3]
 - 1. NNUC No. of nuclides to be printed.
 - 2. NWO WIMS data tape unit no.
 - 3. INEX Inclusive/exclusive print option:
 - 0 = print section if either: nuclide is included in NLIST or section is included in IOUT.
 - 1 = print section only if both: nuclide is included
 in NLIST and section is included in IOUT.
- T Terminate Block 1

Block 2

- Burnup chains 1.
- Burnup chains Fast and resonance groups: σ_p , $\frac{\xi \sigma_s}{\tau}$, σ_{tr} , σ_a , χ , λ 2.
- Fast and resonance groups: $v\sigma_f$, σ_f 3.
- Fast and resonance groups: P scattering matrix 4.
- 5. Thermal temperatures
- Thermal groups: σ_{tr} , α_{a} 6.
- Thermal groups: $v\sigma_f$, σ_f
- Thermal groups: P_0 scattering matrix 8.
- 9. Resonance tables
- P, scattering matrices. 10.
- 3\$ NLIST - List of nuclides to be printed. This list is used together with the values of INEX and IOUT to determine whether a given section of data is to be printed.

т Terminate Block 2

End of Data

Notes:

- SCAN also checks the WIMS tape for errors in structure and unreasonable data values. This checking is performed on the entire tape regardless of whether the data is printed.
- 2. After an update operation, only the nuclides added or edited need be printed. Use NNUC and 3\$ array to select these nuclides, omit the 2\$ array, and set INEX = 0.
- 3. File requirements:

WIMS tape (input).

3.3.4 TRANS

Block 1

- 1\$ Run Parameters [6]
 - 1. NWO - Input WIMS tape unit no.
 - 2. - Output WIMSTAR tape unit no. NWD

 IDTAPE - Identification no. of new WIMSTAR tape (enter 0 if an existing tape is to be extended).

Ò

- 4. NNUC No. of nuclides to be transferred.
- 5. NTE Max. no. of temperatures in resonance tables.
- 6. NSP Max. no. of σ_{p} 's in resonance tables.
- 2\$ List of WIMSTAR identification nos. for the four Pl scattering matrices. Enter 0 for each matrix not required. [4]
- T Terminate Block 1

Block 2 {Repeat NNUC times}

- 3\$ Nuclide Transfer Control [3]
 - NIT NIN from WIMS tape to be transferred. If NIT < 0 transfer is suppressed.
 - 2. IRN Resonance table indicator to be transferred. RIN is generated as RIN = $|NIT| + \frac{|IRN|}{10}$. If $IRN \le 0$ transfer is suppressed.
 - 3. IDN WIMSTAR identification no. of data from NIT.
- T Terminate Block 2

End of Data

Notes:

1. If IDTAPE = 0, the energy group structure of WIMSTAR tape is checked against that of the WIMS tape; then the tape is spaced to the end and the new data is added. If IDTAPE > 0, a new tape is started by placing the energy structure from the WIMS tape on the WIMSTAR tape. When checking the energy structure the program ignores the upper and lower values. However, if a lower value of zero is placed on the WIMSTAR tape, segment GXWIMS will fail when attempting to calculate the lethargy mesh for RESPU. To avoid this problem, do not start a new WIMSTAR tape using TRANS if the WIMS tape has a zero as the lower energy limit.

- 2. If no P1 matrices are required, the 2\$ array is omitted.
- 3. The WIMSTAR identification nos. (IDN) must be unique; if one is duplicated, the data of the second occurrence cannot be used by the update segment. Thus if two sets of resonance tables are required for the same NIN, the 3\$ array is repeated changing IDN. For example:

```
3$ 3238 1 323801 T transfer 3238.1 and 3$ -3238 2 323802 T 3238.2 resonance tables
```

Note that transfer of burnup chain and smooth data is suppressed for the second transfer by using the negative value for NIN 3238.

4. File requirements:

WIMS tape (input)

WIMSTAR tape (output)

3.3.5 TAPMAN

Block 1

- 1\$ Run Parameters [5]
 - 1. IDTAPE Identification no. of the new WIMSTAR tape.
 - NWD Unit no. of the new WIMSTAR tape. Enter 0 to suppress transfer.
 - NTR No. of entries in the record transfer list. Enter 0
 to suppress transfer.
 - 4. NTAPE No. of input WIMSTAR tapes.
 - IOUT Data print flag:
 - -1 = no transfer or listings, produce only a summary of the contents of WIMSTAR tapes.
 - 0 = no listings
 - 1 = list only data written to IDTAPE
 - 2 = list all data read.

T Terminate Block 1

Block 2

- 2\$ List of unit nos. for the input WIMSTAR tapes. [NTAPE]
- 3\$ List of record transfer flags. 0/1 = no-transfer/transfer data
 record. {Required only if NTR > 0.} [NTR]
- T Terminate Block 2

End of Data

Notes:

- 1. The energy structure (NG, N1, N2, N3) of all WIMSTAR tapes processed together must be identical. (Unless IOUT = -1, in which case no processing is done.)
- The length of the 3\$ array should reflect the total number of records from <u>all</u> input WIMSTAR tapes. The list should consist of a set of 0's and 1's (0 = No transfer, 1 = transfer to IDTAPE) which are applied successively to the input records. If the 3\$ list is exhausted, transfer stops; unused elements are ignored.
- 3. To produce tape listings/summaries without writing a new tape:
 - a) To summarize all input tapes with no lists: set IOUT = -1, NWD = 0, NTR = 0, and omit 3\$ array;
 - b) To list all of one or more input tapes: set IOUT = 2, NWD = 0, NTR = 0, and omit 3\$ array;
 - c) To list selected records from one or more tapes: set IOUT = 1, NWD = 0, and use NTR and 3\$ array to select required records.
- File requirements:

WIMSTAR data tape(s) (input)
WIMSTAR data tape (output)

3.3.6 CONVRT

Block 1

- 1\$ Run Parameters [3]
 - 1. ITYPE Conversion direction:

1 = Binary to BCD

2 = BCD to Binary

- 2. NWO Input WIMS tape unit no.
- 3. NWN Output WIMS tape unit no.
- T Terminate Block 1

End of Data

Note:

1. File requirements

WIMS tape (input)
WIMS tape (output)

3.4 JOB CONTROL CONSIDERATIONS

Each of the five AMPX modules required, NPTXS, XLACS2, AJAX, RADE and WIMSTAR-4, has been saved in a separate load module. The AMPX-II driver program has also been saved as a load module. This driver program reads the module request cards and module data cards, initiates execution of each requested module, and prints a summary of the run. The driver program and requested modules are executed via a cataloged procedure called AMPX2. (See the sample case in Appendix C for a listing and use of this procedure.)

```
The procedure is executed via

// EXEC AMPX2,GRGN=400K,GTIME=10,

// U14='&&A',U15='&&B'
```

where GRGN defines the core region in K bytes, GTIME sets the task time limit in minutes, and any of the scratch units 14 through 19 that are required are activated as shown. Each load module required is concatenated to the steplib as

```
//GO.STEPLIB DD

// DD (NPTXS load module)

// DD (WIMSTAR load module)

// DD (XLACS2 load module)

.
.
.
```

Each data file required is also defined to the procedure as

```
//GO.FTnnF001 DD (file description)
```

where nn is the two-digit FORTRAN logical unit number. Finally the card data is entered as

```
//GO.SYSIN DD *
. data cards
.
```

The file requirements and data card input for each module are listed in Section 3.2 for the AMPX-II modules, and Section 3.3 for WIMSTAR. The core region parameter is discussed in the next section. All modules write printed output to unit 6, and if necessary, punched output to unit 7.

3.5 DYNAMIC CORE ALLOCATION

WIMSTAR uses the AMPX system of dynamic core allocation whereby all available core in the user's region is allocated to the program.

The use of this core is dynamically determined at execution time by the

requirements of the specific task. The size required is wholly dependent on the particular nuclide being processed and the processing required. If the size requested through the GRGN parameter of the AMPX2 procedure is insufficient, a WIMSTAR error message is printed (if the system detects this problem, an IHO240I message is printed), and the user simply increases the GRGN specification and reruns the job. WIMSTAR error messages are listed in Appendix A. Each segment of WIMSTAR informs the user of the amount of dynamic core available and, at termination, of the amount of that core that was not used. It is suggested that GRGN initially be set to 400 K and subsequently adjusted as necessary.

NPTXS and XLACS2 use similar core allocation, but the size must be set when the load module is created. For the present implementation the container arrays for NPTXS and XLACS2 were set at 90 000 and 70 000 words respectively, and the modules require 640 K and 540 K regions respectively. The user is directed to the AMPX-II user's manual (4) if these values require adjustment.

AJAX and RADE use the same system as WIMSTAR.

3.6 ERROR PROCESSING

The user is directed to the AMPX-II user's manual (4) to interpret error messages from the AMPX modules.

When WIMSTAR detects an error, the following message is printed:

ERRORERROR CODE n IN SUBROUTINE name

where name is the subprogram detecting the error, and n is the error code number. These codes are explained in Appendix A. A FORTRAN IHO220I error is then intentionally committed to obtain a subroutine traceback to aid in solving the problem. Finally WIMSTAR is terminated with a Run/Completion Code of 16. Some routines print additional information and others print self-explanatory messages.

The current version of the AMPX-II driver program prints the Run/Completion Code when a module terminates, and begins execution of the next module requested, regardless of the value of the previous Run/Completion Code. The user is warned that modules executed subsequent to an abnormally terminated module will probably not run properly if they require results from the errant module. If a system error occurs (illegal operation, illegal core location reference, etc.), everything grinds to a halt, and the AMPX-II driver cannot print the module termination message.

4. PROGRAM MAINTENANCE INFORMATION

This chapter is intended to aid the maintenance programmer in making future modifications to WIMSTAR.

4.1 OVERLAY STRUCTURE

The recommended overlay structure is illustrated in Figure 2, and the subroutines and common blocks contained in each overlay module are listed in Table 3. The function of each module is described below.

- Module 1 Contains the mainline program, input/output routines, error routines, and other service routines required by the rest of the program. This module controls segment execution.
- Module 2 segment WIMLIB
- Module 3 control for segment GXWIMS
- Module 4 multigroup phase of GXWIMS
- Module 5 resonance phase of GXWIMS

Module 6 - segment SCAN

Module 7 - segment TRANS

Module 8 - segment TAPMAN

Module 9 - segment CONVRT

4.2 PROGRAMMING DETAILS

The mainline program reads the segment request cards and calls the appropriate segment driver subroutines. The setup of each segment is essentially the same. Variables to be read through the FIDO input system are collected in common blocks and read by calling FIDAS. The input/output devices must be initialized to assign core space to the buffers. Then all remaining available core is assigned to the segment via the call to the assembler routine ALOCAT. If a routine to allocate core dynamically is not available at a particular installation, the following FORTRAN subroutine may be substituted:

SUBROUTINE ALOCAT (SUB)
COMMON/SPACE/D(50000)
LIMIT = 50000
CALL SUB (D,LIMIT)
RETURN
END

where the length of D is set at compile time. The called subroutine then partitions the D vector into smaller parts as required by the particular task. Upon entry each segment prints the length of the D vector; at termination it prints the amount that was not used during execution of the segment.

Subroutine GMR with its entry points START, END, CLOCK, ENTER and ERROR prints entry, exit, timing and error messages.

The resonance table calculation phase of GXWIMS is performed by RESCAL. Four large work spaces (W1, W2, W3, W4), two smaller work spaces (W5, W6), and three scratch tapes (NT1, NT2, NT3) are used in manipulating point data. The lethargy mesh is generated using $\sigma_{\rm T}$ and $\sigma_{\rm el}$, maintaining $\Delta U_{\rm max}$ as defined in Section 3.3.1, and eliminating all zero value cross sections. The slowing-down equation is solved by RECH2 of module RESPU from the RSYST Code System, for one resonance absorber and one moderator (hydrogen). INTGRC performs the integration to calculate the resonance integral. LAMDA calculates the Goldstein-Cohen λ -values for the first temperature and smallest $\sigma_{\rm p}$. For each successive $\sigma_{\rm p}$ the unresolved resonance region cross sections are replaced, provided a PXS-FD tape is available. The following service subroutines are used to manipulate the point cross sections: ADDXS, COMPRS, EXPAND, LINEAR, MULT, RESINT, RPLCE, and THNFIT. Results are printed, plotted, and written to the WIMSTAR tape by RESOUT.

The multigroup phase of GXWIMS is handled by WIMSXS. TREAD reads the AMPX master library and VECTOR and MATRIX accumulate the required one— and two-dimensional cross sections respectively. WIMS cross sections are calculated as per Section 2.3.1, condensed scattering matrices are generated by WIMFMT, and the results are printed, plotted, and written to the WIMSTAR tape.

UPDATE is the main WIMS library update routine of segment WIMLIB. Each of the four sections—burnup chains, multigroup data, resonance data, and Pl scattering matrices—are updated separately by subroutines BURNUP, SMOOTH, RESON, and PISCAT, respectively. In each case the program compares the NIN and RIN lists input by the user with those on the old tape to determine whether the data is to be added, edited, or deleted. Before each record is written to the new WIMS tape, FIDO input routine FIDAS is called to allow the user to override any item via card input. On option the edited data files are printed.

WIMSCN is the main WIMS tape scan routine which calls subroutine CHECK entry points OCHK, SCHK, VCHK, and PCHK to check NIN order, data sequencing, data values, and condensed scattering matrix structure, respectively. Logical function IO controls printing of selected nuclide files.

Subroutines TRANS3 and TRANS2 handle transfer of data from WIMS to WIMSTAR tapes for resonance tables, and all other data, respectively, in segment TRANS. Subroutine WTAPE2 performs similar functions for segment TAPMAN. SUMARY prints a list of the control records for WIMSTAR tapes. Segment CONVRT uses subroutine BINBCD to perform binary-to-BCD conversion and BCDBIN for BCD-to-binary conversion.

4.3 DATA FILE FORMATS

The user is directed to the ENDF/B user's guide (2) for the format of the ENDF/B library, and to the AMPX-II user's manual (4) for the format of the AMPX master library and the energy group tape. The WIMS library format (taken from Reference (7)) is included here to aid in interpreting the listings produced by the module SCAN.

4.3.1 WIMS Library Format

Introduction

The library tape is composed of a series of files written in the FORTRAN binary mode. There is a general index file, followed by a file for each nuclide giving the basic cross sections, followed by a file for each resonance group giving the temperature and σ_p (effective potential scattering) dependent cross sections for each resonance element.

Each nuclide is identified by a nuclide identification number (NIN); this NIN is in general chosen so that the NIN modulo 1000 is the atomic mass number of the nuclide in question. Each resonance tabulation is identified by the NIN of the nuclide to which it refers together with a single decimal point number (thus any nuclide can have up to 10 - .0, .19 - resonance tabulations associated with it); these combined give the resonance identification number RIN (which is a floating point value, as opposed to the integer value NIN).

The energy groups are counted from high to low energy; similarly, all information is tabulated in order of decreasing energy. A positive distinction is made between fast, resonance and thermal energy groups, the cuts usually being taken as ~ 10 keV and 4 eV, although these figures are quite arbitrary.

General Index File

The first file on the tape contains the following general information:

Record 1: L,N,NO,N1,N2,N3,NNF,NNFP

Number of nuclides on this library tape.

Total number of groups (=N1+N2+N3). Number of groups into which there is a fission source. Numbers of fast, resonance and

٠

Numbers of fast, resonance an thermal groups.

Numbers of fissile and fission product nuclides.

Record 2: (IN(I), I=1, L)

Nuclide identification numbers for the L nuclides on the tape; these form an index to the nuclide files. Record 3: (GB(J), J=1, N+1)

Energy group boundaries - in order of decreasing energy.

Record 4: (FS(J), J=1, NO)

Fission source spectrum, sums to 1.0.

Records 5, JC,JB,(AA(k),

to L+4: JJ(k), k=1,JA)
where JA=JC/2-1 and
may differ for each
record

A record for each nuclide describing all nuclides produced by burnup of this nuclide. This record contains:

Length of record (JC), NIN(JB). Yield (normally 1.0) and NIN of nuclide formed by neutron capture in nuclide JB. Decay constant of nuclide JB and NIN of nuclide formed by decay.

Fission energy yield and indicator NFA (see below). Pairs of numbers giving yield and NIN of fission products produced by fission of JB. Pairs of numbers 0.0 and NIN of any nuclides formed only indirectly from JB (e.g., U^{238} +n+n $\rightarrow Pu^{240}$, Sm^{149} +n $\rightarrow Sm^{150}$, requiring specification of Pu^{240} , Sm^{150} respectively).

The indicator NFA is equal to NF for nuclide JB unless nuclide JB is a fission product; in this case NFA is -1 if nuclide JB does not have a resonance tabulation associated with it, and -2 if it does. If yield and NIN of nuclide formed by capture in nuclide JB are both set to zero, no capture product will be assumed in any subsequent calculation of burnup.

File Mark.

Nuclide Files

For each of the nuclides specified in record 2 of the general index file, there is a file of data containing the following information:

Record 1:/ J,AW,IAN,NF,NT,NZZ

NIN, atomic weight, atomic number, trigger (see below), number of temperatures at which thermal data tabulated, number of resonance tabulations associated with this nuclide.

for fast and resonace

groups.

NF is the fissile and resonance trigger, and may take the following values:

- 0 non-fissile, no resonance tabulation
- 1 non-fissile, resonace absorption tabulation
- 2 fissile, tabulation of resonance absorption only (e.g., Pu^{240})
- 3 fissile, tabulation of resonance absorption and fission
- 4 fissile, no resonance tabulation.

Note that the atomic weight should be exact because it is used in WIMS for calculating number densities from physical densities.

Record 2:	(PSCAT(J), J=1,N2)	$\sigma_{ m p}^{},$ potential scattering cross section, for resonance
		groups.
	(XISS(J),J=1,N2)	$\xi\sigma_{_{ m S}}/ au,$ slowing down power
		divided by lethargy width,
		for resonance groups.
	(TR(J),J=1,N1+N2)	σ_{rr} , transport cross section

(ABS(J), J=1, N1+N2)

 σ_a , absorption cross section for fast and resonance groups.

(CHI(J),J=1,N2)

 χ , for resonance groups, not used beyond WIMSB.

(ALAMDA(J), J=1, N2)

 λ , Goldstein-Cohen parameter, for resonance groups.

Record 3: (XNUFIS(J), J=1, N1+N2), (FIS(J), J=1, N1+N2) $v\sigma_f$ and σ_f , fission yield and fission cross sections for fast and resonance groups.

Record 3 is present only for fissile nuclides (i.e., NF \geq 2). For nuclides with resonance tabulation(s), the resonance group cross sections are 'infinitely dilute' (i.e., no resonance shielding). Note that these cross sections can in general be consistent only with one resonance tabulation.

Record 4: K, (AA(I), I=1, K)

Condensed scattering matrix for scattering from fast and resonance groups.

The vector AA(I) may be split into N1+N2 blocks of the form
AS.AL, (VECTOR(I), I=1,L),

where the numbers in VECTOR are the non-zero scattering cross sections from a group, L=AL is the number of these cross sections, and AS is the position of the self-scatter term in the array VECTOR. Note that AS=1 if there is no upscatter.

Record 5: (TEMP(J), J=1, NT)

Temperatures (K) at which thermal data is tabulated, in ascending order. (If

NT=1 there is one thermal data tabulation, which is then used for all temperatures in WIMS; in this case TEMP(1) is usually arbitrarily set equal to 300 K).

Following this record, there are three records for each temperature as follows:

Record 6: (TR(J), J=N1+N2+1, N),(ABS(J), J=N1+N2+1, N) σ_{tr} and σ_{a} , transport and absorption cross sections for thermal groups (for the appropriate temperature).

 $v\sigma_{f}$ and σ_{f} , fission yield and fission cross sections for thermal groups.

Record 7 is present only for fissile nuclides (i.e., NF > 2).

Record 8: KA, (AA(I), (I=1, KA)

Condensed scattering matrix for scattering from thermal groups. The data are stored as described for record 4.

After the thermal data for all temperatures specified in record 5, data for this nuclide are terminated.

File Mark.

This concludes the description of the L nuclide files 2 to L+1.

Resonance Data Files

The resonance data are contained in N2 files, one for each resonance group. Each file contains one (absorption) or two (absorption and fission yield) records for each resonance tabulation, depending on the trigger NF in the nuclide data of the nuclide to which the tabulation refers. The records are in the order of the NIN's in the index (Record 2, General Index File). The records contain:

```
RIN,M1,M2,(T(JB),JB=1,M1),
(SIGP(JD),JD=1,M2),
((RSIG(JD,JB),JD=1,M2),
JB=1,M1)
```

Resonance identification number, number of temperatures and σ_p 's, temperatures, σ_p 's, and resonance cross sections ordered σ_p within temperature.

Note that the upper value of σ_p in the tabulation is ignored and replaced by 'infinity' when WIMS interpolates in the RSIG table. Following the records for each resonance identification number, the data for each group are terminated by

One record: 0.0, 1, 1, 0.0, 0.0, 0.0 File Mark.

Pl Scattering Matrices

The P_1 scattering matrix data consist of a single P_1 matrix for hydrogen, deuterium, oxygen and carbon in that order. The matrices are written to tape one row at a time; thus the P_1 scattering matrix file consists of 4N records.

System EOF Mark

Some early WIMS tapes do not contain NNF, NNFP, or ALAMDA data items. WIMSTAR-4 cannot process these tapes.

4.3.2 WIMSTAR Data Tape Format

The WIMSTAR tape consists of pairs of records. The first of each pair is a control vector of length 10 that describes the data record that follows it. The format of the burnup chain and scattering matrices is the same as on the WIMS library tape.

1. Tape Control (appears only once as the first pair of records)

Control Record:

- 1. IDR = 1
- 2. IDTAPE identification no. of tape
- 3. NG no. of energy groups
- 4. N1 no. of fast groups
- 5. N2 no. of resonance groups
- 6. N3 no. of thermal groups
- 7.-9. zero
- 10. L length of data record = NG+1

Data Record: (D(I), I=1,L) - energy boundaries.

2. Burnup Chain

Control Record:

- 1. IDR = 2
- 2. IDN nuclide identification no.
- 3.-9. zero
- 10. L length of data record = N.

Data Record: N, (D(I), I=2, N) - burnup chain.

3. Multigroup Data - Fast and Resonance Groups

Control Record: 1. IDR = 3

- 2. IDN nuclide identification no.
- 3. T temperature
- 4.-9. zero
- 10. L length = 4*N1+8*N2

Data Record: $\sigma_p(N2)$, $\xi \sigma_s/\tau(N2)$, $\sigma_{tr}(N1+N2)$, $\sigma_a(N1+N2)$, $\chi(N2)$, $\chi(N$

Note: the values in brackets indicate the length of each cross section.

- 4. Multigroup Data Thermal Groups
- Control Record: 1. IDR = 4
 - 2. IDN nuclide identification no.
 - 3. T temperature
 - 4.-9. zero
 - 10. L length = 4*N3

Data Record: σ_{fr} , σ_{a} , $\nu\sigma_{f}$, σ_{f} (each of length N3)

- 5. PO Scattering Matrix Fast and Resonance Groups
- Control Record: 1. IDR = 5
 - 2. IDN nuclide identification no.
 - 3. T temperature
 - 4.-9. zero
 - 10. L length = N+1

Data Record: N, (D(I), I=1, N) - condensed scattering matrix

6. PO Scattering Matrix - Thermal Groups

The format is identical to record type 5, except that IDR = 6.

- 7. Resonance Table
- Control Record: 1. IDR = 7
 - 2. IDN = nuclide identification no.
 - zero
 - 4. ISF type (1/2 = absorption/fission yiela)
 - 5. NTE no. of temperatures
 - 6. NSP no. of $\sigma_{\rm p}$ values

7.-9. zero

10. L - length = NTE+NSP+(NTE*NSP*N2)

Data Record: (T(I), I=1, NTE), (S(I), I=1, NSP),

(((D(I,J,K),I=1,NSP),J=1,NTE),K=1,N2)

- resonance table data

8. Pl Scattering Matrix

Control Record: 1. IDR = 8

2. IDN - nuclide identification no.

3. T - temperature

4.-9. zero

10. L - length = NG*NG

Data Record: ((D(J,I),J=1,NG), I=1,NG) - P1 scattering data sequenced

"to" within "from" groups.

System EOF mark ends the tape data.

4.3.3 PXS-ID Tape Format

This tape contains infinitely dilute point cross sections for the resolved and unresolved resonance regions.

Record 1: MAT, MF, MT, ZA, AWR, zero, LFS, zero, zero.

Record 2: MAT, MF, MT, T, SIGP, zero, zero, N1, N2,

(NBT(I), INT(I), I=1, N1),

(X(I),Y(I),I=1,N2).

Record 3: MAT, MF, 7 zeros.

Records 1, 2 and 3 are repeated for each MT of MAT.

Record 4: MAT, 8 zeros.

Record 5: 9 zeros.

Groups of records 1-5 are repeated for each MAT on the tape.

System EOF mark.

The variables have the same meaning as for the ENDF/B tapes (see Reference (2)).

4.3.4 PXS-FD Tape Format

This tape contains finitely dilute point cross sections for the unresolved resonance region.

Record 1: 1. ID19 - nuclide identification no.

2. T - temperature

3. SIGP - σ_p value

4.-10. zero

Record 2: $N, (E(I), \sigma_T(I), I=1, N)$

Record 2 is repeated for σ_{el} , σ_{f} , σ_{v} .

Records 1 and 2 are repeated for each $\boldsymbol{\sigma}_{p}\text{,}$ temperature, and nuclide on the tape.

System EOF mark.

e cross sections σ_T , σ_{el} , σ_f , σ_{γ} are total, elastic scattering, ssion, and (n,γ) respectively.

5. SUMMARY

WIMSTAR (Version 4) is a FORTRAN-IV computer program developed for inclusion as a module in the AMPX-II ENDF/B processing system. In conjunction with existing AMPX modules, WIMSTAR provides the capability of generating library data files for the WIMS lattice code and updating the WIMS library tape.

WIMSTAR adheres to the conventions of the AMPX system and can easily be implemented on a computer currently supporting the AMPX system. Several minor modifications to AMPX-II module NPTXS were necessary. AMPX-II currently accesses ENDF/B-IV tapes; modifications to AMPX modules XLACS2 and NPTXS, and to WIMSTAR, will be required when ENDF/B-V is released for general use.

WIMSTAR is divided into six separately executable segments to accomplish data generation, post generation data manipulation, and WIMS tape update and format conversion.

Multigroup cross sections are calculated by AMPX-II module XLACS2 and placed in the WIMS format by WIMSTAR. The major development effort was devoted to resonance processing. The slowing-down equation is solved numerically using point cross sections tabulated on a very fine energy mesh to obtain resonance integrals for the absorber mixed with pure hydrogen.

WIMSTAR can generate all the WIMS data required with the exception of fission source spectra, burnup chain data, and χ . Future improvements could include providing group structure condensation, an upgraded Goldstein-Cohen λ calculation, and better facility for display of cross sections.

6. ACKNOWLEDGEMENTS

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TABLE 1

69-GROUP WEIGHTING SPECTRUM

REGION A (Groups 1 to 14 inclusive)

Energy	Dry 69-Group Weighting Spectrum	Wet 69-Group Weighting Spectrum
11.3315 MeV	0.000077	0.0003
8.82497	0.000288	0.0012
6.87289	0.001082	0.0043
5.35261	0.003415	0.0125
4.16862	0.007253	0.0250
3.24652	0.015299	0.0477
2.52839	0.032235	0.0821
1.96912	0.040766	0.0925
1.53355	0.068804	0.1270
1.19433	0.092740	0.1446
0.930145	0.151457	0.1831
0.724397	0.293853	0.2321
0.564161	0.359617	0.2432
0.439639	0.273385	0.2287
0.342181	0.579860	0.3326
0.266491	0.797033	0.3665
0.207543	1.020714	0.4096
0.161635	1.108708	0.4687
0.125881	1.392871	0.5421
98.0635 KeV	1.538518	0.6346
76.3509	2.025529	0.7520
59.4621	2.256529	0.8839
46.3092	2.717019	1.0847
36.0656	2.929716	1.2975
28.0879	2.913247	1.6002
21.8749	5.728346	2.0012
17.0362	5.345382	2.4685
13.2678	6.613002	3.1004
10.3330	8.260331	3.8690
8.04733	8.314061	4.8358

The first spectrum given above was used as the weighting spectrum for GALAXY in producing the 14 fast groups for every element except hydrogen and oxygen. The latter elements used the second spectrum.

REGION B

In Groups 15 to 56 inclusive the weighting is proportional to ${\rm E}^{-1}$.

REGION C

In Groups 57 to 69 inclusive the weighting is proportional to

$$\frac{1}{(kT)^2}$$
 E_e -E/kT where kT = 2.522 x 10 8 MeV.

This table was taken from Reference (3).

TABLE 2
69-GROUP ENERGY BOUNDARIES FOR WIMS

Group	Energy	Energy Width	Lethargy Width	Group	Energy	Energy Width	Lethargy Width
	MeV				eV		
1	10.0 -6.0655	3.9345	0.49997	28	4.00 -3.30	0.700	0,19237
2	6.0655 -3.679	2.3865	0.49998	29	3.30 -2.60	0.700	0.23841
3	3.679 -2.231	1.448	0.50019	30	2.60 -2.10	0.500	0.21357
4	2.231 - 1.353	0.878	0.50013	31	2.10 -1.50	0.600	0.33647
5	1.353 -0.821	0.532	0.49956	32	1.50 -1.30	0.200	0.14310
6	0.821 -0.500	0.321	0.49592	33	1.30 -1.15	0.150	0.12260
7	0.500 -0.3025	0.1975	0.50253	34	1.15 -1.123	0.027	0.02376
8	0.3025 -0.183	0.1195	0.50260	35	1.123-1.097	0.026	0.02342
9	0.183 -0.1110	0.072	0.49996	36	1.097-1.071	0.026	0.02399
10	0.1110 -0.06734	0.04366	0.49978	37	1.071-1.045	0.026	0.02458
11 12	0.06734-0.04085 0.04085-0.02478	0.02649 0.01607	0.49985 0.49987	38 39	1.045-1.020 1.020-0.996	0.025	0.02421 0.02381
13	0.02478-0.01503	0.01607	0.49987	40	0.996-0.972	0.024	0.02381
14	0.01503-0.009118	0.005912	0.49980	41	0.972-0.950	0.024	0.02289
17	0.01303-0.009110	0.003912	0.49000	42	0.950-0.910	0.040	0.04302
			i	43	0.910-0.850	0.060	0.06821
	eV			44	0.850-0.780	0.070	0.08594
	_			45	0.780-0.625	0.155	0.22154
15	9118.0 ~5530.0	3588.0	0.50006	46	0.625-0.500	0.125	0.22314
16	5530.0 -3519.1	2010.9	0.45198	47	0.500-0.400	0.100	0.22314
17	3519.1 -2239.45	1279.65	0.45198	48	0.400-0.350	0.050	0.13353
18	2239.45 -1425.1	814.35	0.45199	49	0.350-0.320	0.030	0.08961
19	1425.1 - 906.898	518.202	0.45197	50	0.320-0.300	0.020	0.06454
20	906.898 - 367.262	539.636	0.90395	51	0.300-0.280	0.020	0.06899
21	367.262 - 148.728	218.534	0.90396	52	0.280-0.250	0.030	0.11333
22	148.728 - 75.5014			53	0.250-0.220	0.030	0.12783
23	75.5014- 48.052	27.4494		54 5.5	0.220-0.180	0.040	0.20067
24	48.052 - 27.700	20.352 11.732	0.55085 0.55085	55 56	0.180-0.140 0.140-0.100	0.040 0.040	0.25131 0.33647
25 26	27.700 - 15.968 15.968 - 9.877	6.091	0.48038	57	0.100-0.080	0.020	0.33647
20 27	9.877 - 4.00	5.877	0.90391	57 58	0.080-0.067	0.020	0.22314
	9.077 - 4.00	3.077	0.00001	59	0.067-0.058	0.009	0.14425
				60	0.058-0.050	0.008	0.14842
			ł	61	0.050-0.042	0.008	0.17435
			ł	62	0.042-0.035	0.007	0.18232
				63	0.035-0.030	0.005	0.15415
				64	0.030-0.025	0.005	0.18232
			1	65	0.025-0.020	0.005	0.22314
				66	0.020-0.015	0.005	0.28768
			ł	67	0.015-0.010	0.005	0.40547
			Į	68	0.010-7.005	0.005	0.69315
			ĺ	69	0.005-0	0.005	-

TABLE 3

OVERLAY MODULE CONTENTS

					
	Module 1		Module 2	Module 3	
MAIN ALOCAT CORE* CORE2* DATE FIDAS [†] GMR	HDPRNT HEADER* ICONV LIMITS* MESAGE† NWDID PRINT	READ REVS SAVE SETCOR SUMARY WRITE	BURNUP BURN1 FIND FLAGS P1SCAT RESON SMOOTH UPDATE WIMLIB	GXWIMS PPGBW PLOT WXCAL CORE1* GETAP	
Modu	ıle 4		Modu	le 5	
INDEX MATGEN MATRIX MWORD REAL	SIGP TREAD VECTOR WIMSXS WIMFMT	ADDXS ALPHA ANS ANUSET COMPRS DIRINT EMESH	EXPAND INTEGR* INTERP INTGRC ITPOS LAMDA LINEAR	MULT NPTRD RECH2 RESCAL RESINT RESOUT RPLCE	SIALUP SIGSET SIGUP1 SUA1 TERP1 THNFIT ZWEIG1
Module 6	Module 7	Module 8	Module 9		
CHECK IO SCAN SCAN1 WEP WIMSCN	TRANS TRANS1 TRANS2 TRANS3	PRINT1 PRINT2 TAPMAN WTAPE1 WTAPE2	BCDBIN BINBCD CONVRT CONV1		

^{*} Common Block.

t Calls other subroutines of a package not listed here.

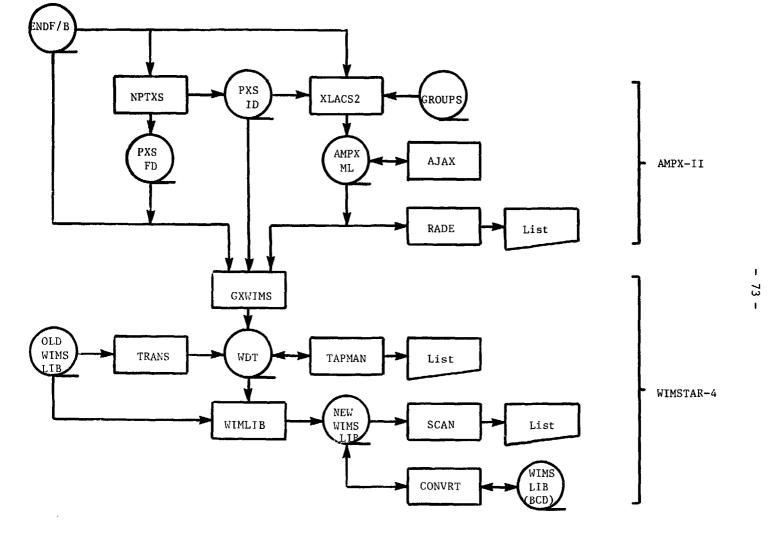
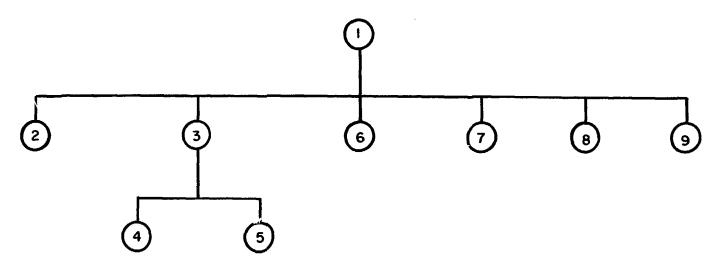


FIGURE 1: AMPX-II/WIMSTAR-4 Organization





Numbers refer to modules of Table 3.

FIGURE 2: Overlay Structure of WIMSTAR-4

APPENDIX A

WIMSTAR ERROR MESSAGES

The error message format is

ERRORERROR CODE n IN SUBROUTINE name

where name is the routine detecting the error, and n is the error code described below. A FORTRAN IHO220I error is then intentionally committed to obtain a subroutine traceback. And finally the program is terminated with a Run/Completion code of 16. Some routines print additional information, and others print self-explanatory messages.

Routine	Error	Description
WIMSTR	1	Illegal segment name.
ADDXS	1	Available core exhausted.+
ANUSET	1	Coefficient limit of 10 exceeded for $\nu(E)$ on ENDF.
	2	Interpolation limit of 5 exceeded for $\nu(E)$ on ENDF.
	3	Point limit of 50 exceeded for $v(E)$ on ENDF.
	4	Request for $v(E)$ outside valid E range.
	5	Invalid interpolation table for $v(E)$ on ENDF.
	6	ENDF read error: MF=1, MT=452, LNU out of range.
BURNUP	1	3\$ array read error.
	2	ID3 < 0 not allowed for new nuclide.
	3,4	10*, 14* array read error.
	5	Problem with burnup chain edit data, check order
		and content of NIN lists.

See footnote on page 79.

Routine	Error	Description
BURN1	1	Problem with 14* burnup chain edit input, cannot find referenced NIN.
CONVRT	1	1\$ array read error.
	2	ITYPE invalid, must be 1 or 2.
EMESH	1	Available core exhausted.+
FIND	1	Invalid WIMSTAR tape unit no.
	2	Can't find WIMSTAR record: NT = unit no., IDN =
		nuclide identifier, IT = record type, T = temperature,
		ISF = resonance table type.
FLAGS	1	Invalid data source for new nuclide.
	2	Invalid NIN detected.
	3	Invalid RIN detected.
GETAP	1	Can't find a resonable value for APA.
GXWIMS	1	1\$ array read error.
	2	2\$ array read error.
	3	Temperature or σ_p limit exceeded: NTE ≤ 10 and NTE+NSP ≤ 20 .
	4	3*,4*,5* array read error.
	5	6\$ array read error.
	6	Program error: WIMSTAR tape structure invalid.
	7,8,9,	Energy structure does not match existing WIMSTAR
	10	tape: 7/8/9/10 = Total/Fast/Resonance/Thermal.
LAMDA	1	Group structure doesn't match point data.
NPTRD	1	Interpolation limit of 25 exceeded on NXS tape.
	2	Available core exhausted. +
	3	Temperature on NXS tape does not match 4* array entry
		for nuclide ID19.

⁺ See footnote on page 79.

Routine	Error	Description
	4	NXS tape problem: invalid $\sigma_{\rm p}$ detected.
PPGBW	1	No NAM tape and energy structure not card input.
	2	NAM tape has wrong no. of groups.
PISCAT	1	NWO and NEP are inconsistent.
	2	6\$ array read error.
	3	10* array read error.
	4	NEP must equal 0 or 4.
RESCAL	1	Can't find correct point data on NXS tape.
	2	Available core exhausted. +
	3	AWA invalid.
	4•	Incorrect temperature on data from NSD tape.
RESON	1	WIMS tape problem in resonance tables.
	2,3,4	Problem with resonance table edit data, check RIN's;
		or program error.
	5	10\$, 11*, 12* array read error.
	6	Available core exhausted. +
	7	13* array read error.
	8,9	Problem with resonance table edit data, check RIN's.
	10	5* array read error.
RPLCE	1	Energy range of NSD tape does not match that of NXS
		tape.
SCAN	1	1\$ array read error.
	2	2\$,3\$ array read error.
SIGSET	1	Can't find material MAT on ENDF tape.
SMOOTH	1	4* array read error.
	2,6	Problem with smooth edit control data, check NIN
		lists for order and content.

⁺ See footnote on page 79.

Routine	Error	Description
	- 3	Error in reading one of: 10*,11*,12*,13*,14*,15*, 16*,17*,23*,24\$,25\$,26* arrays.
	4	Attempt to change no. of temperatures invalid.
	5	Error in reading one of: 18*,19*,20*,21*,26*
		arrays.
SUMARY	1	Program error: WIMSTAR tape structure invalid.
TAPMAN	1	1\$ srray read error.
	2	2\$,3\$ array read error.
TERP1	1	Interpolation code out of range.
	2	Zero or negative value can't be interpolated by logs.
TRANS	1	1\$,2\$ array read error.
	2	Program error: WIMSTAR tape structure invalid.
	3,4,	Energy structure on WIMS tape does not match existing
	5,6	WIMSTAR tape: 3/4/5/6 = Total/Fast/Resonance/Thermal.
TRANS2	1	Group boundaries on WIMS tape don't match existing
		WIMSTAR tape.
	2	Maximum no. of thermal temperatures (20) exceeded.
	3	3\$ array read error.
TRANS3	1	NTE exceeded.
	2	NSP exceeded.
	3	WIMS tape problem: fission flag (NF) not consistent
		with resonance tables.
	4	WIMS tape problem: resonance tables not complete.
UPDATE	1,4,5,6	Available core exhausted.+
	2	8\$,9\$,10*,11* array read error.
	3	Group boundaries on WIMSTAR tape don't match old
		WIMS tape.

^{*} See footnote on page 79.

Routine	Error	Description
WIMLIB	1	0\$,1\$,2\$ array read error.
	2,3,4,5	Input energy structure does not match old WIMS tape:
		2/3/4/5 = Total/Fast/Resonance/Thermal.
	6	Program error: WIMSTAR tape structure invalid.
	7,8,9,10	Input energy structure does not match WIMSTAR tape:
		7/8/9/10 = Total/Fast/Resonance/Thermal.
WIMSXS	1,2,4,5,	6 Available core exhausted. ⁺
	3	Insufficient data on AMPX Master Library tape.
	7	Energy boundaries don't match.
	8	Can't find requested nuclide on AMPX Master Library
		tape.
	9	9* array read error.
WIMFMT	1	Available core exhausted. +
WTAPE2	1,4	Energy boundaries don't match on all input WIMSTAR
		tapes.
	2	Available core exhausted. +
	3	Program error: WIMSTAR tape structure invalid.
WXCAL	1,2	Available core exhausted. +
	3,4	Energy group structure input does not match AMPX
		Master Library tape.
	5	7*,8* array read error.

⁺ Increase the REGION size on the job step EXEC card and rerun the step. Not all uses of dynamic core can be checked beforehand.

[Eg., READ(1)K, (A(I), I=1,K)]. If there is not enough space in one of these cases, an IHO240I error occurs accompanied by a Run/Completion code of SOC1. Increase REGION and rerun the step.

APPENDIX B

FIDO INPUT SYSTEM

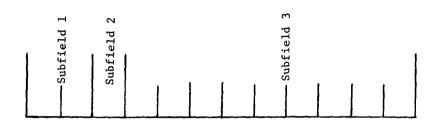
The FIDO input method is especially devised to allow the entry or modification of large data arrays with minimum effort. Special advantage is taken of patterns of repetition or symmetry wherever possible. The FIDO system was patterned after the input method used with the FLOCO coding system at Los Alamos and was first applied to the DTF-II code. Since that time, numerous features requested by users have been added, a free-field option has been developed, and the application of FIDO has spread to innumerable codes. This description was taken from Reference (4) of the main text.

The data are entered in units called "arrays". An array comprises a group of contiguous storage locations which are to be filled with data at one time. These arrays usually correspond on a one-to-one basis with FORTRAN arrays used in the program. A group of one or more arrays read with a single call to the FIDO package forms a "block", and a special delimiter is required to signify the end of each block. Arrays within a block may be read in any order with respect to each other, but an array belonging to one block must not be shifted to another block. The same array can be entered repeatedly within the same block. For example, an array could be filled with "O" using a special option, and then a few scattered locations could be changed by reading in a new set of data for that array. If no entries to the arrays in a block are required, the delimiter alone satisfies the input requirement.

Three major types of input are available: fixed-field input, free-field input, and user-field input.

Fixed-Field Input

Each card is divided into six 12-column data fields, each of which is divided into three subfields. The following sketch illustrates a typical data field. The three subfields always comprise 2, 1, and 9 columns, respectively.



To begin the first array of a block, an <u>array originator field</u> is placed in any field on a card:

Subfield 1: An integer array identifier < 100 specifying the data array to be read in.

Subfield 2: An <u>array-type</u> indicator:
"\$" if the array is integer data,
"*" if the array is real data.

Subfield 3: Blank

Data are then placed in successive fields until the required number of entries has been accounted for.

In entering data, it is convenient to think of an "index" or "pointer" which is under control of the user and which specifies the position in the array into which the next data entry is to go. The

pointer is always positioned at array location #1 by entering the array originator field. The pointer subsequently moves according to the data operator chosen. Blank fields are a special case in that they do not cause any data modification and do not move the pointer.

A data field has the following form:

- Subfield 1: The <u>data numerator</u>, an integer < 100. We refer to this entry as N_1 in the following discussion.
- Subfield 2: One of the special data operators listed below.
- Subfield 3: A nine-character data entry, to be read in F9.0 format. It will be converted to an integer if the array is a "\$" array or if a special array operator such as Q is being used. Note that an exponent is permissible but not required. Likewise, a decimal is permissible but not required. If no decimal is supplied, it is assumed to be immediately to the left of the exponent, if any, and otherwise to the right of the last column. This entry is referred to as N₃ in the following discussion.

A list of data operators and their effect on the array being input follows:

"Blank" indicates a single entry of data. The data entry in the third subfield is entered in the location indicated by the pointer, and the pointer is advanced by one. However, an entirely blank field is ignored.

"+" or "-" indicates exponentiation. The data entry in the third field is entered and multiplied by 10^{\pm} N₁, where N₁ is the data numerator in the first subfield, with the sign indicated by the data

operator itself. The pointer advances by one. In cases where an exponent is needed, this option allows the entering of more significant figures than the blank option.

"&" has the same effect as "+".

"R" indicates that the data entry is to be repeated ${\rm N}_1$ times. The pointer advances by ${\rm N}_1$.

"I" indicates linear interpolation. The data numerator, N_1 , indicates the number of interpolated points to be supplied. The data entry in the third subfield is entered, followed by N_1 interpolated entries equally spaced between that value and the data entry found in the third subfield of the next nonblank field. The pointer is advanced by $N_1 + 1$. The field following an "I" field is then processed normally, according to it 3 own data operator. The "I" entry is especially valuable for specifying a spatial mesh. In "\$" arrays, interpolated values will be rounded to the nearest integer.

"L" indicates logarithmic interpolation. The effect is the same as that of "I" except that the resulting data are evenly separated in log-space. This is especially convenient for specifying an energy mesh.

"Q" is used to repeat sequences of numbers. The length of the sequence is given by the third subfield, N_3 . The sequence of N_3 entries is to be repeated N_1 times. The pointer advances by $N_1 * N_3$. If either N_1 or N_3 is 0, then a sequence of $N_1 + N_3$ is repeated one time only, and the pointer advances by $N_1 + N_3$. This feature is especially valuable for geometry specification.

The "N" option has the same effect as "Q", except that the order of the sequence is reversed each time it is entered. This is

valuable for the type of symmetry possessed by \mathbf{S}_{n} quadrature coefficients.

"M" has the same effect as "N" except that the sign of each entry in the sequence is reversed each time the sequence is entered. For example, the entries:

1 2 3 2M2

would be equivalent to

1 2 3 -3 -2 2 3.

This option is also useful in entering quadrature coefficients.

"Z" causes $\mathrm{N}_1^{}+\mathrm{N}_3^{}$ locations to be set to 0. The pointer is advanced by $\mathrm{N}_1^{}+\mathrm{N}_3^{}$,

"C" causes the position of the last array item entered to be printed. This is the position of the pointer, less 1. The pointer is not moved.

"0" causes the print trigger to be changed. The trigger is originally off. Successive "0" fields turn it on and off alternately. When the trigger is on, each card image is listed as it is read.

"S" indicates that the pointer is to skip N_1 positions leaving those array positions unchanged. If the third subfield is blank, the pointer is advanced by N_1 . If the third subfield is nonblank, that data entry is entered following the skip, and the pointer is advanced by $N_1 + 1$.

"A" moves the pointer to the position, $\mathbf{N}_{\mathbf{3}},$ specified in the third subfield.

"F" fills the remainder of the array with the datum entered in the third subfield.

"E" skips over the remainder of the array. The array length criterion is always satisfied by an E, no matter how many entries have been specified. No more entries to an array may be given following an "E", except that data entry may be restarted with an "A".

The reading of data to an array is terminated when a new array origin field is supplied or when the block is terminated. If an incorrect number of positions have been filled, an error edit is given; and a flag is set which will later abort execution of the problem. FIDO then continues with the next array if an array origin was read. Otherwise, it returns control to the calling program.

A <u>block termination</u> consists of a field having "T" in the second subfield. All entries following "T" on a card are ignored, and control is returned from FIDO to the calling program.

Comment cards can be entered within a block by placing an apostrophe (') in column 1. Then columns 2-80 will be listed, with column 2 being used for printer carriage control. Such cards have no effect on the data array or pointer.

Free-Field Input

With free-field input, data are written without fixed restrictions as to field and subfield size and positioning on the card. The options used with fixed-field input are available, although some are slightly restricted in form. In general, fewer data cards are required for a problem, the interpreting card is easier to read, a card listing is more intelligible, the cards are easier to keypunch, and certain common keypunch errors are tolerated without affecting the problem.

Data arrays using fixed- and free-field input can be intermingled at will within a given block.

The concept of three subfields per field is still applicable to free-field input, but if no entry for a field is required, no space for it need be left. Only columns 1-72 may be used, as with fixed-field input.

The <u>array originator field</u> can begin in any position. The array identifiers and type indicators are used as in fixed-field input. The type indicator is entered twice, to designate free-field input (i.e., "\$\$" or "**"). The blank third subfield required in fixed-field input is not required. For example:

31**

indicates that array 31, a real-data array, will follow in free-field format.

Data fields may follow the array origin field immediately. The data field entries are identical to the fixed-field entries, with the following restrictions:

- Any number of blanks may separate fields, but at least one blank must follow a third-subfield entry if one is used.
- If both first- and second-subfield entries are used, no blanks may separate them, i.e., 24S, but not 24 S.
- 3. Numbers written with exponents must not have imbedded blanks, i.e., 1.0E+4, 1.0E4, 1.0+4, or even 1+4, but not 1.0 E4.
- 4. In third-subfield data entries, only nine digits, including the decimal but not including the exponent field, can be used, i.e., 123456.89E07, but not 123456.789E07.

- 5. The Z entry must be of the form: 738Z, not Z738 or 738 Z.
- 6. The + or data operators are not needed and are not available.
- 7. The Q, N, and M entries are restricted: 3Q4, 1N4, or M4, but not 4Q, 4N, or 4M.

User-Field Input

If the user follows the array identifier in the array originator field with the character "U" or "V", the input format is to be specified by the user. If "U" is specified, the FORTRAN FORMAT to be used must be supplied in columns 1-72 of the next card. The format must be enclosed by the usual parentheses. The data for the entire array must follow on successive cards. The rules of ordinary FORTRAN input as to exponents, blanks, etc., apply. If the array data do not fill the last card, the remainder must be left blank.

"V" has the same effect as "U" except that the format read in the last preceding "U" array is used.

APPENDIX C

SAMPLE CASE

This appendix contains the input for a sample case to illustrate some of the features of the AMPX/WIMSTAR system. The output from WIMSTAR is available from the author on request. A sample of the output from NPTXS and XLACS2 can be found in the AMPX-II user's manual (from Reference 4 of main text).

NPTXS and XLACS2 were run to generate point and multigroup cross sections for $^{232}\mathrm{Th}$ at 300 K and 9 values of σ_p . Nuclide identification no. 129601 was used. Next GXWIMS calculated the WIMS data and placed it on a new WIMSTAR tape 800226 under identification no. 23202. TRANS transferred current $^{232}\mathrm{Th}$ data from NIN 1232 of an old WIMS tape to identification no. 23201 of the same WIMSTAR tape. Then WIMLIB added the new version of $^{232}\mathrm{Th}$ to the WIMS tape using NIN 2232 and RIN 2232.1, using the old burnup chain, and the new multigroup and resonance data. The new WIMS tape was then scanned for errors and finally converted to BCD for shipment.

```
// EXEC AMPX.GRGN=640K.GTIME=30.U14='&&A'.U15='&&B'.U16='&&C'.
// U17='&&D',U18='&&E',U19='&&F'
//STEPLIB DD
// DD
         (NPTXS LOAD MODULE)
// DD
         (XLACS2 LOAD MODULE)
// DD
         (WIMSTAR LOAD MODULE)
//FT01F001 DD (OLD WIMS LIBRARY)
//FT11F001 DD (ENDF/B TAPE)
//FT23F001 DD (AMPX MASTER LIBRARY)
//FT31F00! DD (POINT X-SECTIONS, INFINITE DILUTION)
//FT41F001 DD (POINT X-SECTIONS, FINITE DILUTIONS)
//FT47F001 DD (ENERGY GROUP LIBRARY)
//FT50F001 DD (NEW WIMS LIBRARY, BCD FORMAT)
//SYSIN DD *
=NPTXS
1$$ 1 T
2$$ 1296 A4 2 9 129601 3** A4 300 T
4## 1+6 10500 3208 1662 842 392 162 102 52 T
=XLACS2
AMPX2 IBM STANDARD VERSION
XLACS2
TH232 MAT 1296 (USING NPTXS DATA)
300K 69 GROUPS
FISS-1/E-MAX WEIGHTING
1$$ 1 1 69 42 2 2$$ A2 11000 26000 A8 2 E 3$$ F1 T
8## 300 5 1,27+6 67,4+4 E T
TH232 MAT 1296 (USING NPTXS DATA)
70$$ 129601 1296 1 3 3 A7 -2 E 71** 1+6 A5 129601 31 0 0 129601 T
73** 300. T
=WIMSTAR
GXWIMS CAL. TH232 DATA
1$$ 1 T
2$$ 11 17 0 801111 1296 23202 1 9 69 14 13 42 2 3 1 500 T
3## 0 11.2 232.0381 0 0.01
4** 300
5** 52 102 162 392 842 1662 3208 10500 1+6 T
6$$ 129601 23 31 41 1 2 0 0 T
<sup>3</sup>## F0.2 T
TRANS TH232 WIMS TO WIMSTAR
1$$ 1 17 0 1 3 10 T
3$$ 1232 3 23201 T
TAPMAN CHECK LIST TH232
1$$ A4 1 -1 T
2$$ 17 T
```

FIGURE C.1: Sample Case - Input

```
WIMLIB UPDATE TH232
0$$ 0
1$$ 1 18 17 25 1 1 1 0
2$$ 94 69 27 14 13 42 13 37 T
8$$ 2001 6001 2002 8002 3 4 6 7 9 10 1010 11 12 1012 2012 2212
    14 16 19 23 27 29 52 55 56 1056 58 63 2063 91 93 112 83 95 99
    101 1103 103 105 1105 108 109 113 115 127 131 133 134 135 1135
    143 145 147 1147 2147 148 1148 149 150 151 152 153 154 155 1155
    157 164 902 176 178 181 207 232 1232 2232 9233 1233 234 235 1235 236
    237 3238 939 3239 1240 241 242 941 942 943 1000 2000 1999
9** 232.1 1232.1 1232.2 1232.3 2232.1 9233 9233 1233 234 235.2 235.2
    235.3 235.4 235.4 235.4 1235.2 1235.2 1235.3 1235.3 1235.4 1235.4
    236 3238.5 3239.1 3239.1 T
3$$ 2232 23201 O T
4** 2232 23202 300 232.0381 90 2 1 1 0 T
23## 300 T
5** 2232.1 23202 1 0 0 T
     WIMS TAPE FOR ERRORS.
SCAN
1$$ 0 18 0 T
2$$ FO T
CONVRT BINARY TO BCD
1$$ 1 18 50 T
/*
11
```

APPENDIX D

INPUT SUMMARIES

This appendix contains summaries of the input requirements discussed in Section 3. It is intended as a quick reference after the user becomes familiar with the complete instructions.

TABLE D.1

AMPX-II INPUT SUMMARY

Ma J., 1	Module Block	Array		Data		
модите	Block	No.	Length	Data		
NPTXS	1	0\$	1	broadening method		
		1\$	1	NNUC		
	2	2\$	6	MATNO, NDFB, IDTAP, MODE, NSIGP, ID19		
		3*	4	RFACT, SFACT, SIGP, TDEGIC		
	3	4*	NSIGP	σ values (only if NSIGP > 1)		
	1	Repeat	Blocks 2	and 3 NNUC times		
XLACS2	1			Five title cards		
	2	1\$	5	ID, NNUC, MAXG, NEG, IW		
		2\$	12	LSLAB, LCYL, LUNR, MSN, NPE, NPEP, IDTAP, MODE,		
				NGMA, LCSM, MCSM, NDNP		
		3\$	6	output flags		
	3	4\$	IDTAP	ENDF MT identifiers for punched cross section		
		5\$	2xLCSM	interpolation scheme for weighting spectrum		
		6*	2xMCSM	weighting spectrum		
		7*	MAXG+1	energy group boundaries, decreasing		
		8*	10	T, χ, THETA, FCUT, 6 entries not used		
				One title card		
	4	70\$	9	ID19, MATNO, NTEMP, LORDER, NL, NFY, MATID,		
				кмхв, кмха		
		71*	9	SIGP, AJIN, RFACT, SFACT, MATPT, NUNIT, MME,		
				MMI, MATEL		
	5	73*	NTEMP	temperatures, increasing		
	H	Repeat	title ca	rd and Blocks 4 and 5 NNUC times		
XALA	1	0\$	2	MMT , NMAX		
•		1\$	1	NFILE		

TABLE D.1, concluded

Block			- Data
2	2\$	2	NF,IOPT
3	3\$	IOPT	list of nuclide identifiers added or
			deleted
	4\$	IOPT	list of new nuclide identifiers (only if
			change required)
	Enter 1	Block 3	only if IOPT ≠ 0
	Repeat	Blocks	2 and 3 NFILE times
1	1\$	4	MMT, 3 entries not used
	2\$	20	IOPT1, IOPT2, 18 entries not used
	2 3	2 2\$ 3 3\$ 4\$ Enter 1 Repeat	2 2\$ 2 3 3\$ IOPT 4\$ IOPT Enter Block 3 Repeat Blocks 1 1\$ 4

TABLE D.2
WIMSTAR INPUT SUMMARY

Segment	Block	lock Array		Data	
		No.	Length	Data	
GXWIMS	1	1\$	1	NNUK	
	2	2\$	16	NDF, NWD, IOUT, IDTAPE, MAT, IDN, NTE, NSP, NG, N1,	
				N2,N3,IFL,IFR,IFP,NWK	
	3	3*	5	DUMAX, SIGPA, AWA, APA, ERR	
		4*	NTE	temperatures, increasing	
		5 *	NSP	$\sigma_{\mathbf{p}}^{}$, increasing	
	4	6\$	8	ID19, NAM, NXS, NSD, ITFP, ITFT, ITFO, ITF1	
		Repeat	Block 4	NTE times	
	5	7*	N2	λ	
		8*	NC+1	energy group boundaries (only if no AMPX	
				tapes)	
	:	Input	Block 5 o	nly if IFP=1	
	6	9*	NGxN1	$\sigma_{ m TR}^{}$ weights	
	1	Repeat	Block 6	for each ITFT=3 or 5	
	1	Repeat	Blocks 2	-6 NNUK times	
VIMLIB	1	0\$	1	IOUT	
		1\$	8	NWO, NWN, NWD, LRIN, NEB, NES, NER, NEP	
		2\$	8	LNIN, NG, NO, N1, N2, N3, NNF, NNFP	
	2	8\$	LNIN	nuclide identification nos.	
		9*	LRIN	resonance table identification nos.	
		10*	NG+1	energy group boundaries	
		11*	NO	fission source spectrum	
	3	3*	3	NIN3, ID3, LENB	
	4	10*	LENB	burnup chain	
	7				
	4	14*	LENB x3	burnup chain edit control	

TABLE D.2, continued

Segment	Bloc	k No.	Array Length	Data
	5	4*	9	NIN4, ID4, TFR, AW, IAN, NF, NT, NZZ, NP4
	6	10*	N 2	σ p
		11*	N2	ξσ _s /τ
		<u>12*</u>	N1+N2	o TR
		<u>13*</u>	N1+N2	σ a
		14*	N2	x
		<u>15*</u>	N2	λ
		<u>16*</u>	N1+N2	^{νσ} f
		<u>17*</u>	N1+N2	$\sigma_{\mathbf{f}}$
		26*	NP4	condensed fast and res. P scat. matrix
		23*	NT	thermal temperatures
		24\$	NT	lengths of thermal P scat. matrices
		25\$	NT	Block 7 input flags (one per temp.)
	7	18*	м3	^σ TR
		<u>19*</u>	N3	σ a
		<u>20*</u>	N3	νσ _f
		<u>21*</u>	N3	$^{\sigma}\mathbf{f}$
		26*	24\$	condensed thermal P_o scat. matrices
		Repeat	Block 7	for each 1 in 25\$
		Repeat	Blocks 5-	-7 NES times
	8	5*	5	RIN5, ID5, ISF, NTE, NSP
	9	10\$	N2	Block 10 input flags (one per res. group)
		11*	NTE	temperatures, increasing (only if ID5=0)
		12*	NSP	$\sigma_{\rm p}$, increasing (only if ID5=0)
	10	13*	NTEXNSP	resonance table, σ_{p} within temperature
	:	Repeat	Block 10	for each 1 in 10\$
		_	_	-10 NER times
		-		!

TABLE D.2, concluded

Segment	Block	Array No. Length		Data							
	11	6\$	1	ID6							
	12	10*	NGxNG	P ₁ scat. matrix, "to" within "from" groups							
		Repeat Blocks 11 and 12 NEP times									
SCAN	1	1\$	3	NNUC, NWO, INEX							
	2	2\$	10	data section print flags							
		3\$	NNUC	nuclide identification no. print list							
TRANS	1	1\$	6	NWO, NWD, IDTAPE, NNUC, NTE, NSP							
		2\$	4	P_1 scat. matrix WIMSTAR identification list							
	2	3\$	3	NIT, IRN, IDN							
		Repea	t Block 2	2 NNUC times							
TAPMAN	1	1\$	5	IDTAPE, NWD, NTR, NTAPE, IOUT							
	2	2\$	NTAPE	input WIMSTAR tape unit nos.							
		3\$	NTR	record transfer flags							
CONVRT	1	1\$	3	ITYPE, NWO, NWN							

TABLE D.3 MODULE INPUT/OUTPUT REQUIREMENTS

	Module												
Unit Number or					WIMSTAR								
Input Variable Name	NPTXS	XLACS2	AJAX	RADE	GXWIMS	WIMLIB	SCAN	TRANS	TAPMAN	CONVRT			
	10	Ι0	10	10	10	Ι0	I O	Ι0	10	I O			
5 6 11 12 14 15 16 17 18 19 23 31 41 47 MMT NF NAM NXS NSD NDF NWD NWD NWO NWN	C P E S S S S S S F F	C P E T S S S S S G	C P S S S S A A	C P S S	C P S S S S S	C P S S	C P	C P	C P	C P			

I = input

0 = output

A - AMPX master library

C - card reader

E - ENDF/B (fast)

F - PXS-FD (finite dilution)

G - group boundaries tape

I - PXS-ID (infinite dilution)

L - WIMS library tape

P - printer

S - scratch tape

T - ENDF/B (thermal)

W - WIMSTAR data tape

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